UNIVERSITÀ DEGLI STUDI DI BARI
ALDO MORO

DIPARTIMENTO INTERATENEO DI FISICA "M. MERLIN"

Dottorato di ricerca in FISICA – Ciclo XXX

Settore Scientifico Disciplinare FIS/02

Quantum boundary conditions

Dottorando:
Dott. Giancarlo Garnero

Supervisore:
Ch.mo Prof. Paolo Facchi

Coordinatore:
Ch.mo Prof. Gaetano Scamarcio

FINAL EXAM 2017

Imaginé poder tener el universo en un cajón.

Contents

Introduction

Quantum boundary conditions emerge in the description of bounded quantum systems. The analysis of a physical system, indeed, usually discriminates the behaviour of the bulk from the surrounding environment. In this sense, boundary conditions are a crucial ingredient, interpreting the interaction between confined systems and the environment.
Boundary conditions are ubiquitous in every area of physics. For example, there is a large class of problems involving a flow across the interface of two separate media. In this case it is essential to postulate a sort of continuity condition at the interface of the two media.
An example is provided by a sound wave trespassing a tube, whose cross section may abruptly change. In this case, one requires that, where the change occurs, there would be a continuity condition across the junction in the pressure of the air disturbance. Thus, a boundary condition imposes a fundamental restriction on the evolution for the system under consideration. Similar situations may happen for electromagnetic fields at an interface. When a wave enters a region and it encounters a boundary then, the propagation of the disturbance is modified. Indeed, instead of a single progressive plane wave in one direction, one finds waves in both directions. In this case the continuity conditions estabilish a precise distribution of the energy in the reflected and transmitted flux.
A slightly different example is provided by the vibrating string when its ends are held fixed. In this case the condition of no motion at the ends is precisely a continuity condition at the boundary. Incidentally, this condition is important because it introduces discreteness into the motion of the system. Indeed, the so called Dirichlet boundary conditions for the vibrating string limit the possible frequencies of simple harmonic vibrations in the string. Though the former example belongs to the realm of classical physics, it assumed an unforeseen importance already in the very early formulation of quantum mechanics.
Indeed a free quantum particle on an impenetrable segment satisfies a wave-like equation, the Schrödinger equation, and the discrete frequencies repre-

sent the energetic levels of the system.
Moreover, in physics, dynamics is usually expressed in terms of differential equations, which are solvable under various boundary conditions. Indeed, the dynamics of a bounded system requires information on the physical properties of the material the boundary is made of.
In this framework we also find the aforementioned Schrödinger equation, which encodes the dynamics of a nonrelativistic closed quantum system.
In the operatorial description of quantum mechanics, self-adjoint operators are used to describe physical observables.
In some cases, physical reasoning gives a formal expression for the Hamiltonian and other observables as operators on a particular realization of the Hilbert space such as $L^2(M)$, M being the configuration space.
Most physical operators are unbounded so we need to consider the domains where they are defined. Usually, one starts looking for some symmetric operator and tries to check whether it is essentially self-adjoint or not. In the negative case, then, one is forced to study various self-adjoint extensions.
Moreover, in the spirit of the Stone theorem [RS75], self-adjoint operators can be interpreted as the infinitesimal generators of the admissible transformations on the Hilbert space of physical states. For this reason unitarity plays a stringent role in the evolution of the system. From a physical perspective, it translates into the principle of conservation of probability, which imposes that no net loss of probability may occur in a closed quantum system.
This work is divided into five chapters. In chapter 1 we start off with an overview on the main topic of this thesis: quantum boundary conditions. In this chapter we motivate the ubiquitousness of quantum boundary conditions in the physical sciences. We emphasize, both on the classical and the quantum side, the effective role they play in the modeling of physical phenomena, ranging from electrostatics to acoustics, from thermodynamics to nonrelativistic quantum mechanics.
Next, We delve into the analysis of the Casimir effect [Cas48]. Two conducting plates in the vacuum can attract each other even if electrically neutral. We discuss how the choice of certain boundary conditions can alter the force between the plates, which can be shown to be repulsive or even null [AM13; AGM06]. The analysis is conducted on scalar fields and all the physical ingredients can already be found on stage.
We move on to another field where quantum boundary conditions have shown their relevance. It has been proposed that topology change in quantum gravity may be explained in terms of modifications of the boundary conditions in a early Universe [SWX12]. In fact, it has been proposed that space time should not be considered as an immutable entity, rather as something transforming under the laws of quantum mechanics. For this reason, we implement

topology change mechanisms [Bal+95] by means of transforming boundary conditions and show that these are entropy-increasing processes.
Next, we jump on to solid state physics and the quantum Hall effect. In 1980, K. von Klitzing [KDP80] discovered new fascinating scenarios in the Hall effect due to quantum behaviours. In particular, he observed the quantization of electrical resistances in a MOSFET at low temperatures. Furthermore it has been largely studied the connection between the quantum Hall effect and the quantum boundary conditions to be imposed at the edges of the system [QT87; IMT96; Akk+98]. In particular we focus on the modelization of the edge currents, emerging as a boundary effect.
The Aharonov-Bohm effect [AB59] is the last example of quantum boundary conditions provided in Chapter 1. The presence of a magnetic field in a Young experiment with electrons causes a shift in the interference pattern. A solenoid in the Aharonov-Bohm effect induces a perturbation in the configuration space crossed by the electrons, which can be encoded by means of boundary conditions [OP10]. We also discuss how different boundary conditions generate different scattering cross sections, which can be experimentally detected. With this idea in mind, then, one could understand which kind of interaction can occur between the electrons and the solenoid, because mostly it is not clear what boundary conditions can be realized in laboratories. The first chapter ends with a brief overview on the mutual connection between self-adjointness and quantum boundary conditions and a physical interpretation in terms of scattering processes. In particular we give a look at the parametrization of the self-adjoint extensions of the free quantum particle Hamiltonian in terms of unitary operators.
In chapter 2 we get to the heart of the matter revealing the interrelation between geometric phases and quantum boundary conditions. Specifically we consider the case of a nonrelativistic free quantum particle confined into a one dimensional box, whose walls can change in time [Di +16]. We focus on a class of boundary conditions, which are consistent with the symmetries of the system. Time-dependent boundary conditions problem are, in general, very hard to tackle because the vector describing the system samples different Hilbert spaces.
The boundary conditions chosen allow us to map the time-dependent problem into a fixed domain one, where the whole set of computations for the Berry phase can be led.
Interestingly, we find a non-trivial Berry phase in a setting different from the one proposed by M. Berry [BW84]. Moreover the simplest model of hyperbolic geometry emerges, adding an intrinsic geometrical flavour to the evolution. Eventually we present some physical realizations and experimental proposal of geometrical phases.

In chapter 3, we analyze another dynamical problem involving boundary conditions. Indeed, time dependent problems offer a wide range of applications from atoms in cavities to ions trapped in microwave cavities. In this chapter we focus on an evolution à la Trotter. In other words we consider a free quantum particle in an n-dimensional cavity with alternating boundary conditions.
The physics inside the cavity is rapidly interchanged and we investigate the emerging dynamics. The limiting dynamics can be encoded in a composition law for the boundary conditions we started with. We start our analysis with the one-dimensional formulation of the problem [Aso+13] and highlight some of the features, which can be found even in the higher dimensional case. Eventually, we generalize the one-dimensional case and give a final expression for a composition law of boundary conditions inside the cavity.
In chapter 4 we analyze a different aspect involving quantum boundary conditions. In particular, we try to understand how to generate physical systems settled on a manifold with boundaries starting from spaces without boundaries. We are going to check that this can be achieved in different ways. First of all we start with the case of a particle on a circle and after modding it out by the parity action we obtain a free particle on an interval. We investigate the emerging boundary conditions and analyze further generalizations. In the second part, instead, we consider a different procedure. As a matter of fact we start from specific examples and implement folding procedures. For example, for a free quantum particle on the line, we fold the real line in two copies of a half-line, which involves the doubling of the Hilbert space, or in other words the introduction of an auxiliary space. This procedure unitarily introduces a boundary in the system. We reconsider the case of a free particle on a circle and fold the circle in two copies of a segment, doubling the Hilbert space. In light of this doubling we discuss the relation between entanglement and self-adjoint extensions of the Hamiltonians considered. We generalize the examples studied framing them into a general framework. Eventually the chapter ends with a discussion of Naimark's theorem and generalized self-adjoint extensions, where we prove that every symmetric operator admits a minimal extension with the introduction of an ancillary space.
In the last chapter, we describe the mathematical techniques behind the topics we dealt with in the previous chapters. In particular, we investigate the case of a free quantum particle in a cavity Ω. The Hamiltonian describing such a system is an unbounded operator and a precise knowledge of its domain is necessary. Self-adjointness is a fundamental ingredient both from a mathematical and a physical point of view, since it is essential for describing quantum observables.
Moreover we classify all the possibile self-adjoint extensions of the aforemen-

tioned Hamiltonian, comparing with the known results in literature. Eventually, we add some more ingredient on the form-representation theorem, which links self-adjoint operators and quadratic forms. All the results discussed are followed by the respective proofs.

Chapter 1

Quantum Boundary Conditions: an overview

In this chapter we are going to introduce the reader to the role of boundary conditions in Physical Sciences. In particular we will dwell on the quantum realm, testing some phenomena where boundary conditions are not just a mathematical construction but rather a physical key to understand the physics playing behind.
In order to motivate the study of quantum boundary conditions we will discuss about the Casimir effect and the quantum Hall effect, stressing the role played by quantum boundary conditions. Then, we will continue this review with an analysis of topology change in quantum gravity and with the Aharonov-Bohm effect. A concise mathematical motivation of quantum boundary conditions will be given. The chapter ends with a physical interpretation of boundary conditions with a scattering approach.

1.1 Quantum Boundary Conditions

Boundary conditions emerge as an effective description of a physical system with its environment. In particular, when dealing with confined systems, boundary conditions encode the information about the interaction between the system and the rest of the universe through its boundary.

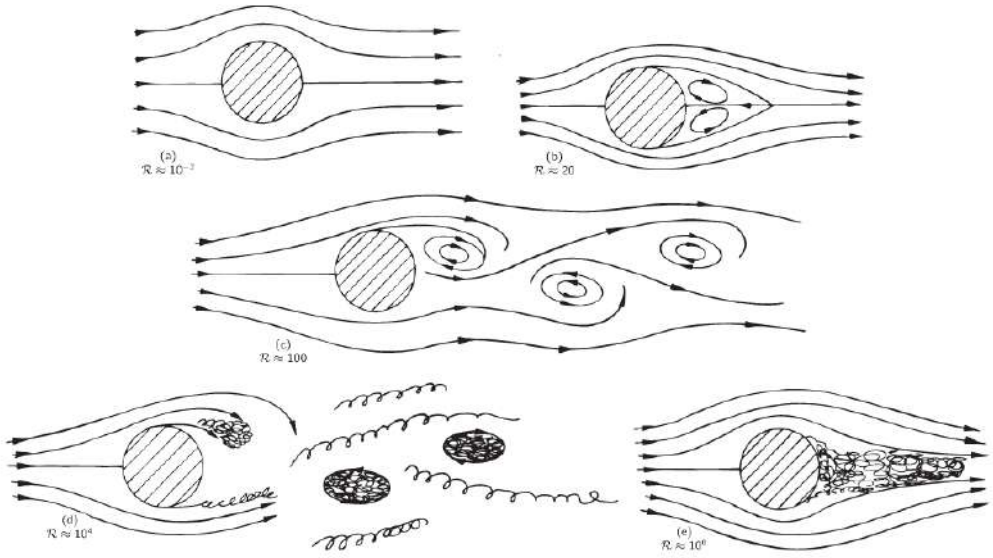

Figure 1.1: The introduction of a cylinder in the flow of a fluid perturbs the configuration of the flow's lines. Here depicted the flow past a cylinder for various Reynolds numbers [FLS70].

Skimming through the *The Feynman Lectures on Physics* [FLS70] can provide an idea of the ubiquitous presence of boundary conditions already at the classical level. They range from the reflection and refraction of light, to waves in dense materials, from viscosity problems to the sounds produced by the strings of a violin or by a drum. These problems usually emerge as *boundary value problems*. A typical example from Electrostatics [Jac98] is the evaluation of the the electrostatic potential Φ in the vacuum generated by a distribution of charges on some conductors; namely one has to solve the Laplace equation with a certain boundary configuration g:

$$\begin{cases} -\Delta\Phi = 0 & \text{in } \Omega \\ \Phi = g & \text{on } \partial\Omega \end{cases}, \tag{1.1}$$

where Ω is the vacuum space among the conductors.
It is well known that the solutions of this problem highly depend on the boundary conditions g and on the geometry of the conductors. There can be, in fact, a plethora of different physical situations ranging from the potential

generated by a single conducting sphere, to the potential generated by a plane, or by a conducting plane with a hole.
They all mathematically translate into the resolution of a partial differential equation with boundary conditions [Eva10], and make use of different techniques like the Green function, the method of images or variational approaches.
The Laplace equation describes a static situation. Clearly, something more can be done studying dynamical equations like the heat equation or the wave equation. For example, the heat equation settled in a region of the space, say $\Omega \subset \mathbb{R}^3$ reads:

$$\partial_t u(t,x) - D\Delta u(t,x) = f(t,x) \qquad x \in \Omega\,,\, t > 0, \tag{1.2}$$

where D is a constant. This equation describes, for example, the evolution of the temperature u of a body confined in Ω under the source term f. Just like the previous case we could think of measuring the temperature on the boundary of the region Ω, or the thermal flux through it, which means that we need to know the behaviour at the boundary at any time.
In any case, since this is an evolution problem in order to know the temperature at any time $t > 0$ we will also need to know the initial temperature.
The heat equation can also be used to study some very basic phenomena in the dynamics of populations. Indeed, suppose that a population is confined in a one dimensional environment $[0, L]$. Very roughly if the population was not confined in this space it would be subject to an exponential growth according to the Malthus model, namely:

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t,x) = a\, u(t,x), \tag{1.3}$$

which admits an exponential solution with $a > 0$. Yet people may tend to escape from crowded regions (e.g. under adverse climatic conditions), and this fact translates into a diffusion term in the evolution equation. Moreover, we suppose that the external environment is ostile. This statement can be translated with the use of boundary conditions, namely $u(0) = 0 = u(L)$.

Thus, the population density at time $t > 0$, at the point x reads:

$$\begin{cases} \partial_t u(x,t) - D\Delta u(x,t) = a\, u(x,t) & x \in (0,L)\,,\ t > 0, \\ u(0,t) = u(L,t) = 0 & t > 0, \\ u(x,0) = u_0(x) & x \in (0,L), \end{cases} \tag{1.4}$$

where u_0 is the population density at $t = 0$.
Moving on to the wave equation, it is well known that the profile u of a plucked string or membrane satisfies the equation:

$$\partial_t^2 u(x,t) - c^2\Delta u(x,t) = f(x,t) \qquad x \in \Omega\,,\ t > 0, \tag{1.5}$$

where c represents the velocity of propagation of the perturbation. In order to study the evolution of the membrane one needs to fix the behaviour at the boundary and the initial data (in this case even on the the velocity since we are dealing with a second order differential equation).
Interestingly, the wave equation in one dimension can be used to determine the pitches of musical notes. Indeed, consider an elastic homogeneous string held strongly at its extremes ($u(0,t) = u(L,t) = 0$), which can be plucked and makes very tiny oscillations with respect to the equilibrium configuration. Then, its shape at time $t > 0$ in x has to satisfies the problem:

$$\begin{cases} \partial_t^2 u(x,t) - c^2\Delta u(x,t) = 0 & x \in (0,L)\,,\ t > 0, \\ u(0,t) = u(L,t) = 0 & t > 0, \\ u(x,0) = u_0(x) & x \in (0,L), \\ \partial_t u(x,0) = v_0(x) & x \in (0,L), \end{cases} \tag{1.6}$$

where u_0 and v_0 are respectively the initial configuration and the initial velocity. One could have used different boundary conditions, for example Neumann boundary conditions:

$$\partial_x u(0,t) = 0 = \partial_x u(L,t), \tag{1.7}$$

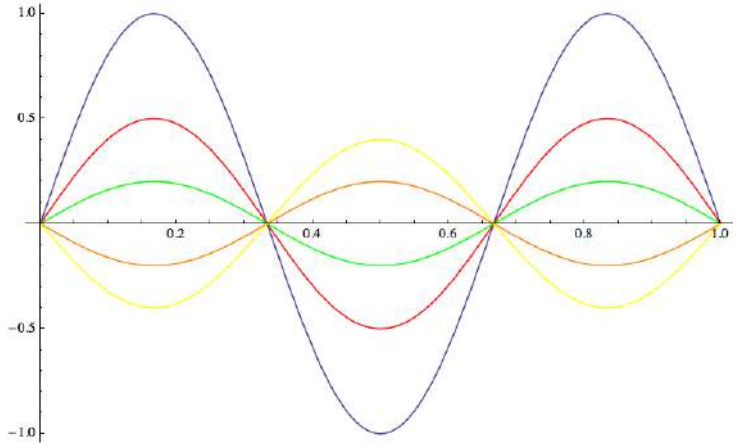

Figure 1.2: Here reproduced at distinct times the different shapes of $u_3(x,t)$ for a string of length 1.

which physically means that each end point is not held fixed, but rather can slide vertically without friction [Min+06a].
It can be proved that the solution of the problem in equation (1.6) is:

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t), \tag{1.8}$$

$$u_n(x,t) = \sin\left(\frac{n\pi x}{L}\right)\left[a_n \cos\left(\frac{n\pi c\, t}{L}\right) + b_n \sin\left(\frac{n\pi c\, t}{L}\right)\right], \tag{1.9}$$

where a_n and b_n are uniquely determined by the initial conditions. Here we are not going to discuss the right hypotheses of convergence of the series, for further details see [Fol09]. From a physical perspective each function $u_n(x,t)$ represents a vibrational motion of the string, also known as *stationary vibration*. Every element of the string evolves periodically in time with a frequency $n\pi c/L$. Moreover the frequency associated to u_n is n times the frequency of u_1, which is the *fundamental frequency* of the string.
For example the vibrating string could be a string of a guitar. From a musical point of view the fundamental frequency represent the pitch of the note we are listening to and its multiples, the higher harmonics, other octaves and notes.
Thus, given a certain initial condition, the real motion of a string is a sum of

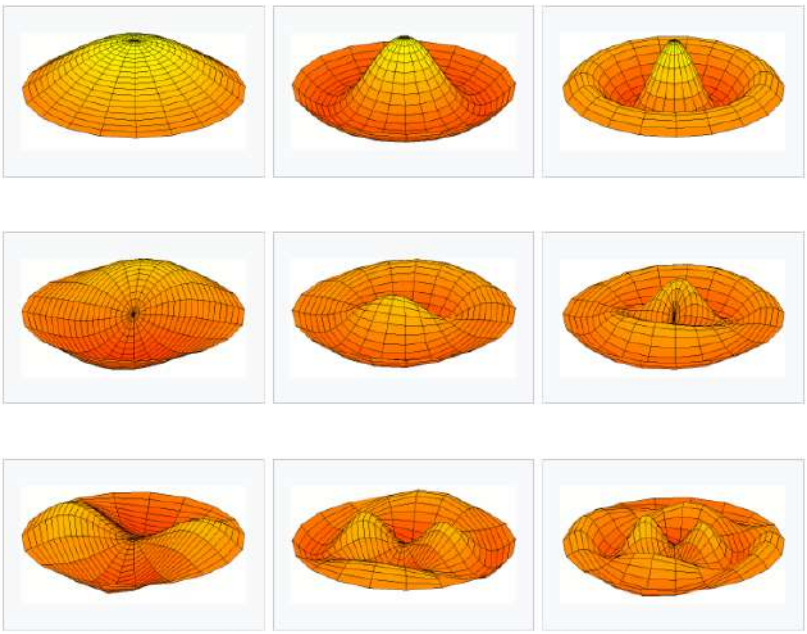

Figure 1.3: Some of the fundamental frequencies of a circular membrane with Dirichlet boundary conditions.

an infinite number of stationary vibrations, which can be well approximated by a finite number of them. For this reason a plucked string usually makes a sound given by a certain fundamental frequency and other harmonics, whose amplitudes have a less important contribution, which make up the timbre of that sound.

For example, in Figure 1.2 the instantaneous shapes of u_3 are shown. In particular, the string vibrates up and down but for the end points of the string and the internal nodes. These characteristics can be found also for a vibrating membrane and its fundamental frequencies (see Figure 1.3). In particular we refer the reader to [Kac66] for and interesting reading on these topics and on how to characterize the oscillation modes with respect to the shape of the membrane.

It is fundamental to remark that all this discussion heavily relies on the structure of the wave equation and on the boundary conditions imposed.

Up to now we have only analyzed the role of boundary conditions in a classical situation. Boundary conditions show their relevance both classically and

quantumly. Take for example a classical particle bouncing against a wall. The dynamics of the particle cannot be described solely by the Hamiltonian function:

$$H = \frac{p^2}{2m}, \tag{1.10}$$

where p represents the particle's momentum and m its mass. Indeed, the expression in equation (1.10) does not provide information on what happens when the particle bounces against the wall.

In order to treat the bouncing back one needs to provide further information about the elastic properties of the material the wall is made of. For example, the particle could scatter elastically, meaning that it reverses its momentum but the kinetic energy is conserved, or could have a sticky reflection, in which case the particle loses energy in the bouncing back process. In the most extreme case the particle could even stop and stick on the wall.

The region on the boundary interested in the reflection of the particle is local, and only a small part of the wall is interested in the dynamics of the collision. So, what can be understood is that the bouncing is described phenomenologically, that is in terms of the elastic properties of the material and is an extra ingredient to the theory.

There is a crucial difference between quantum and classical boundaries. In the mechanical situation of a single particle bouncing back on a wall, only a tiny part of the wall is physically involved in the process. The analogous situation in quantum mechanics is different. Indeed, the wavefunction associated to the particle satisfies the Schrödinger equation, which represents an example of wave equations. For this reason, the *whole* wall, that is the whole boundary, is involved in the bouncing process, and not only a small part of it.

First of all, when we promote the Hamiltonian function to an operator we naively obtain:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{1.11}$$

where $\hbar$ is the Planck constant. Unfortunately, unless one specifies the domain where the former operator acts, it is not possible to determine whether

H could represent a good Hamiltonian and eventually determine a quantum unitary dynamics.
As we are going to revise in section 1.6, observables in quantum mechanics are represented by self-adjoint operators and, in particular, the self-adjointness condition for the operator is encoded in the choice of suitable boundary conditions.
Thus, in quantum mechanics the boundary behaviour is encoded in the Hamiltonian and in the conservation of probability, in other words in *unitarity*. These assumptions are based on physical principles and are much more stringent than those from classical physics.
Interestingly, boundary conditions play an intriguing role not only in nonrelativistic quantum mechanics, but in quantum field theory as well. In fact, there is a plethora of physical systems involving, for example, photons and electrons in a cavity, which can be studied in terms of quantum fields on a bounded domain [AGM15].
In the next sections we are going to discuss some relevant physical situations where boundary conditions play a prominent role. In particular we are going to start with a discussion of the Casimir effect, then consider models of topology change which could be useful in quantum gravity. Eventually the quantum Hall effect and the Aharonov-Bohm effect will be discussed, stressing the role and the relevance of the quantum boundary conditions.

1.2 The Casimir effect

In this section we are going to discuss a physical situation where quantum boundary conditions play a prominent role, the Casimir effect. In 1948 [Cas48] H.B.G. Casimir proved that two conducting plates in the vacuum can attract each other even if electrically neutral. This apparently paradoxical situation can be explained in terms of quantum fluctuations of the ground state of the fields confined between the two plates.
In the original formulation, Dirichlet boundary conditions were imposed for the electromagnetic field on the plates, which, in other words, meant for the fields to vanish on the conducting plates.

In Quantum Field theory the vacuum energy of the fields, that is the energy of the ground state, is ill defined unless one introduces a normal ordering procedure on the operators [Wei05]. Wick's prescription, in fact, forces the subtraction of the infinite value of the vacuum energy, so that the expectation value of the Hamiltonian operator in the ground state is zero.
We are usually interested in differences of energy, which let us a certain freedom in the choice of the origin of energy scales. Casimir proved that a proper definition of the ground state energy requires the knowldege of the interaction of the fields with its environment. Indeed, experimentally, one usually deals with confined systems, so that one can arrange the interaction of the fields with the surrounding constraints in terms of boundary conditions. For this reason, the vacuum energy is defined as the difference between the energy of the ground state for confined fields and the one for free fields, after a proper regularization. Then, a change in the boundary conditions on the system induces a change in the vacuum energy.
As already said, in the first formulation, Casimir made use of Dirichlet boundary conditions, which physically correspond to a zero tangential component for the electric fields on the boundary, as one would expect for a couple of conducting plates. The overall effect predicted was an attractive force between the two plates, due to an increase of the vacuum energy with the distance between the plates.
The phenomen was first observed in 1957 [Spa57], later confirmed under different setups [Bla+60; Sil66; TW68; SA73] and more recently in [Lam97; MR98]. Besides the attractive behaviour it was shown also that, under different configurations, the plates could even repel each other [MCP09].
For the sake of concreteness we are going to discuss how different boundary conditions affect the vacuum energy for a free scalar field [AM13; AGM06]. We are going to consider a static space-time, say $\mathcal{M} = \mathbb{R}\times M$, where $M \subset \mathbb{R}^n$ is a bounded set with regular boundary ∂M. In other words, we are assuming that there is a temporal coordinate globally defined. Moreover, since we will be mainly interested in the Casimir effect, it is not restrictive to consider $M = \mathbb{R}^{n-1} \times [0, L]$, whose boundary is $\partial M = \mathbb{R}^{(n-1)} \times \mathbb{R}^{(n-1)}$. With the above assumptions the Hamiltonian operator describing a free massles scalar

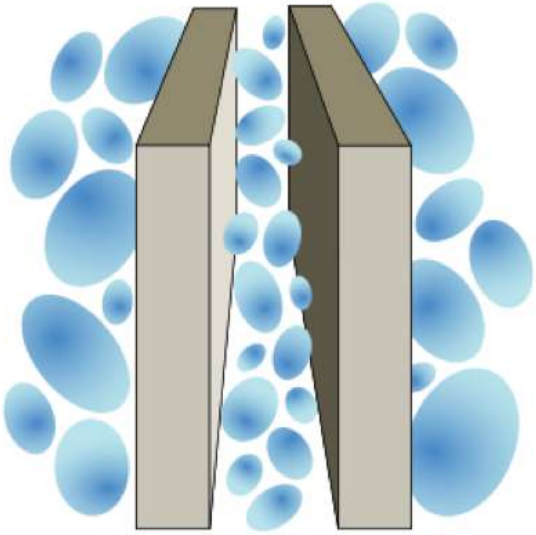

Figure 1.4: Two parallel plates, with their boundary conditions, affect the vacuum fluctuations.

field ϕ is [Wei05] :

$$H = \frac{1}{2}\int_M \left(\pi(\boldsymbol{x})^\dagger \pi(\boldsymbol{x}) + \phi(\boldsymbol{x})^\dagger L_U \phi(\boldsymbol{x})\right) \mathrm{d}\boldsymbol{x}, \tag{1.12}$$

where:

$$L_U = -\frac{1}{2}\Delta_U + \frac{1}{2}m^2, \tag{1.13}$$

Δ_U, being a self-adjoint realization of the Laplace operator determined by a unitary matrix U and $\pi(\boldsymbol{x})$ is the conjugate momentum associated to the field ϕ. For the mutual relation between self-adjoint extensions of the Laplace operator and unitary matrices we refer to the extensive discussion in Chapter 5. As a matter of fact, not all the unitary matrices can be used, rather a subset of them, which is compatible with the symmetries of the system. Moreover we recall that the following commutation relation holds: $[\pi(\boldsymbol{x}), \phi(\boldsymbol{x}')] = -i\hbar\delta(\boldsymbol{x} - \boldsymbol{x}')$ for all $\boldsymbol{x} \neq \boldsymbol{x}'$.
It can be proved that the vacuum energy associated to the scalar field ϕ is:

$$E_U = \frac{1}{2}\mathrm{tr}\, L_U^{\frac{1}{2}}, \tag{1.14}$$

which evidently diverges as long as L_U is not a trace-class operator. Renormalization theory can be invoked in order to cure this divergent contribution. We are not going to enter these details. To the curious reader we recommend [AM13].

If we restrict our attention to the $1+1$ dimensional case, we are considering a field theory on the interval $[0, L]$. Then, different unitary matrices will implement different boundary conditions for the vacuum energy. For example, if one considers periodic boundary conditions for the field, say $\phi(0) = \phi(L)$, then, the vacuum energy reads:

$$E_p = -\frac{\pi}{3L}. \tag{1.15}$$

Instead for Dirichlet ($\phi(0) = 0 = \phi(L)$) or Neumann boundary conditions ($\phi'(0) = 0 = \phi'(L)$) we get:

$$E_{D/N} = -\frac{\pi}{12L}. \tag{1.16}$$

In both cases the vacuum energy is increasing with L, which corresponds to an attractive force between the plates. Nevertheless one could consider pseudo periodic boundary conditions $\phi(L) = \mathrm{e}^{-i\alpha}\phi(0)$, $\phi'(L) = \mathrm{e}^{-i\alpha}\phi'(0)$, which can be obtained with the unitary matrix:

$$U = -\begin{pmatrix} 0 & \mathrm{e}^{i\,\alpha} \\ \mathrm{e}^{-i\,\alpha} & 0, \end{pmatrix} \tag{1.17}$$

where $\alpha \in [-\pi, \pi]$. In this case the vacuum energy reads:

$$E_{pp}(\alpha) = \frac{1}{2L}\left(|\alpha| - \frac{\alpha^2}{2\pi} - \frac{\pi}{3}\right). \tag{1.18}$$

Interestingly this expression can take positive and negative values as well as it could even be zero (see Figure 1.5). For this reason, for certain configurations of the plates there could be no Casimir effect, when the energy is zero, or even a repulsive force between the plates, when the energy is positive, as experimentally observed in [MCP09].

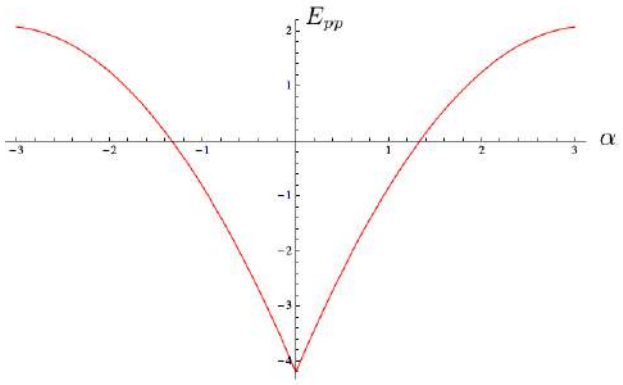

Figure 1.5: Here depicted the dependance on the parameter α of the vacuum energy with pseudo periodic boundary conditions [AGM06].

For simplicity we only focused on a free massless scalar field in a one-dimensional box. The previous discussion can be extended to higher dimensions and, according to the evenness or oddness of the dimension, one can have different behaviours for the vacuum energies.
Moreover, it can be proved that the most intense attractive force between the two plates is achieved when periodic boundary conditions are imposed at the boundary. In this case the vacuum energy attains its minimum value. On the contrary the strongest repulsive effect between the two plates is attained with anti-periodic boundary conditions, which correspond to the maximum value for the vacuum energy.
Before concluding, it is relevant to stress the role of the boundary conditions in the dynamical Casimir effect as well.
When the boundaries are moving, in fact, the force exerted on the walls can be dissipative [Bar93]. As a result, the dissipated energy is used to create real particles inside the cavity. For example, in the context of the dynamical Casimir effect, time dependent boundary conditions can generate photons inside a microwave cavity.
Indeed, it has been proposed that parametric processes can be observed in a system where a boundary condition of the electromagnetic field can be changed in time. The dynamical Casimir effect can be mapped to the quantum version of a parametric oscillator in special cases, which can exist in a

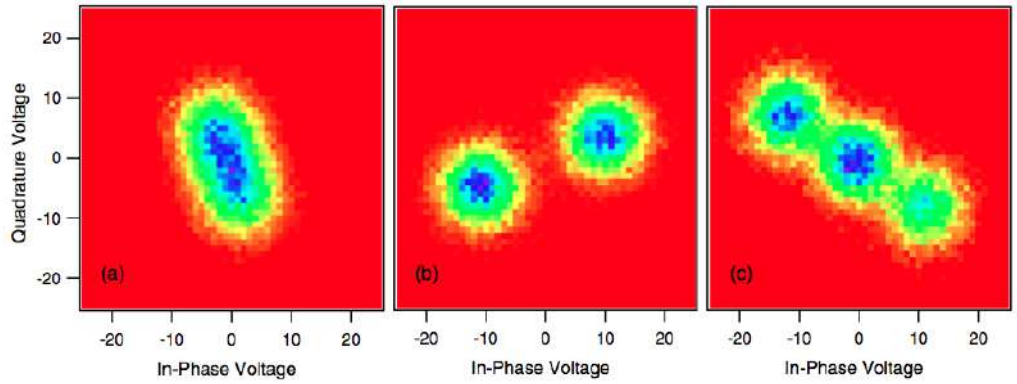

Figure 1.6: Stable states inside a microfabricated quarter-wave coplanar waveguide cavity. For further details about the experiment we refer to [Wil+10].

number of stable dynamical states (See Figure 1.6).
In [Wil+10] they find a good agreement between the response of a cavity with a time dependent boundary condition and the theory of a parametric oscillator. Moreover, the quantitative agreement is good evidence that the source of photon generation is the time dependent boundary. Of course, all these ingredients are highly dependent on the boundary conditions imposed on the walls, as studied in [AFM03; Min+06b; Min+06a; SE06]. Application of the Casimir effect with a gravitational perspective and making use of curved boundaries are to be found in [SS10]. For further readings on the Casimir effect we highly recommend the review [PMG86]

1.3 Topology change and quantum boundary conditions

In this section we are going to review some applications of quantum boundary conditions in the realm of quantum gravity and topology change. For more details see the survey [Aso+12] and references therein.
Notwithstanding more than a century has passed from the theoretical foundations of quantum mechanics and general relativity, it has not been clarified yet how space-time topology is supposed to enter the foundations of a quan-

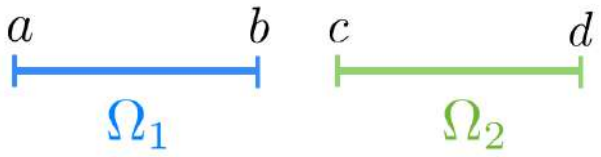

Figure 1.7: Two disjoint intervals as configuration space of a topology change.

tum theory. Some suggestions may come from quantum gravity and the spin-statistics connection. Indeed, it has been proposed that the texture of space-time could be considered as something alive which can shape itself under the laws of quantum mechanics.

Apparently the unfolding of classical topology from the quantum realm is a very subtle point as proved by the vast literature in the field, for example see [Bal+83; Bal+91].

There is a general belief that a quantum version of gravity should be consistent with the spin-statistics theorem. It seems reasonable that a change in the topology of space-time could emerge due to spin-statistics connection related to geons. As a matter of fact, geons emerge as solitonic excitations of twisted spatial manifolds. A change in the topology of space-time is necessary in order to get pair production or annhilation of geon and antigeon, the antiparticle of a geon.

It is well known, for example, from relativistic quantum theories that a spin-statistics connection is present in theories which admit creation and annhilation processes [Wei05]. Seemingly a quantum theory of gravity may not be compatible with some sort of spin-statistics theorem unless a change in the topology is admitted.

With this aim in mind, in 1995 [Bal+95] some simple quantum models were investigated. In particular, it was shown how a change in the classical underlying topology can happen even in elementary quantum physics.

Here we are going to briefly recall some of the main results on topology change shown in the paper. Let us consider two disjoint intervals, say $\Omega_1 = (a, b)$ and $\Omega_2 = (c, d)$, with $a < b < c < d$, and define the composite space Ω as the union of the two intervals, say, $\Omega = \Omega_1 \cup \Omega_2$, as shown in Figure 1.7.

From a physical point of view we are considering a free quantum non-relativistic particle which lives in Ω and which can tunnel, for example, from the point b to the point c. All the possible interactions and linkings between the endpoints are expressed in terms of boundary conditions, as we are going to recall.

Let us fix a Hilbert space $\mathscr{H} = L^2(\Omega)$ and consider the Hamiltonian operator describing a free particle:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{1.19}$$

where m is the mass of the particle and $\hbar$ the Planck constant. From a mathematical point of view this operator is unbounded and, as such, it needs to be settled on some suitable domain in $\mathscr{H}$. In particular, the Hamiltonian operator represents a physical observable, say the energy of the system, and, as such, it has to be a self-adjoint operator, as prescribed by one of the axioms of Quantum Mechanics.

For example, one could start from $D(H) = C_0^\infty(\Omega)$, the set of regular functions with compact support in Ω. On this domain the operator is only symmetric and not self-adjoint. Nevertheless the operator in equation (1.19) is a good candidate for a physical observable. So one looks for the self-adjoint extensions of this operator. In order to do so one considers the boundary form:

$$\Gamma(\psi, \phi) = \langle \psi, H^*\phi \rangle - \langle H^*\psi, \phi \rangle \tag{1.20}$$

and looks for all the possible boundary conditions that make the latter form vanish. Indeed, after integrating by parts:

$$\Gamma(\psi, \phi) = \left[\overline{\psi'(x)}\phi(x) - \overline{\psi(x)}\phi'(x)\right]_{\partial\Omega} \tag{1.21}$$

is expressed in terms of the boundary values of the wavefunctions. It can be proved [AIM05] that every possible (self-adjoint) physical realization of the problem is uniquely determined by a unitary matrix, say $U \in \mathrm{U}(4)$. In particular, fixed a unitary matrix U, then the corresponding domain of

self-adjointness for H is:

$$D(H_U) = \{\psi \in H^2(\Omega) : \ \mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}\},$$

where φ and $\dot{\varphi}$ are the boundary data of the wave function ψ and are defined as

$$\varphi := \begin{pmatrix} \psi(a) \\ \psi(b) \\ \psi(c) \\ \psi(d) \end{pmatrix}, \qquad \dot{\varphi} := \begin{pmatrix} -\psi'(a) \\ \psi'(b) \\ -\psi'(c) \\ \psi'(d) \end{pmatrix}. \tag{1.22}$$

where the minus signs, which appear in the $\dot{\varphi}$ vector, are chosen such that the normal vector field on $\partial\Omega$ points outward. We recall that $H^2(\Omega)$ is the Sobolev space of square integrable functions ψ with square integrable first and second derivative, respectively ψ' and ψ''. For the mathematical details we refer to Chapter 5.
Moreover, any wave function ψ in the domain of H_U satisfies the boundary conditions

$$\mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}. \tag{1.23}$$

For example, the unitary matrix:

$$U_1 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{1.24}$$

generates the following boundary conditions:

$$\begin{cases} \psi(a) = \psi(d), \\ \psi(b) = \psi(c), \\ \psi'(a) = \psi'(d), \\ \psi'(b) = \psi'(c). \end{cases} \tag{1.25}$$

which corresponds to a connected single circle (Figure 1.8).

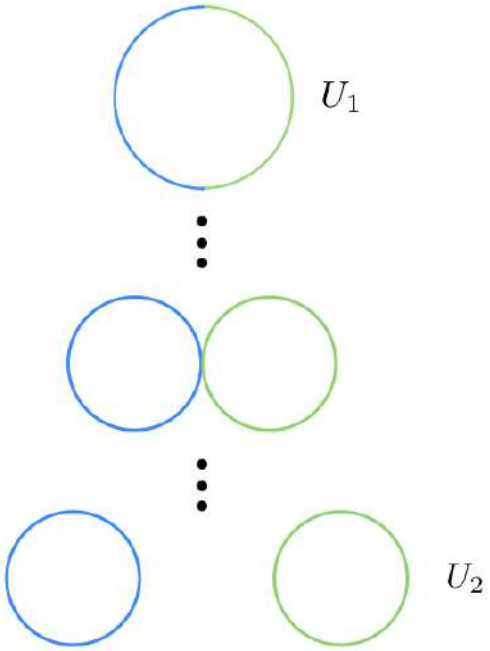

Figure 1.8: Interpolation between different topologies determined by distinct boundary conditions.

While the matrix:

$$U_2 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \tag{1.26}$$

determines a different behaviour at the boundary, say:

$$\begin{cases} \psi(a) = \psi(b), \\ \psi(c) = \psi(d), \\ \psi'(a) = \psi'(b), \\ \psi'(c) = \psi'(d), \end{cases} \tag{1.27}$$

which corresponds to the topology of a couple of disconnected circles. (Figure 1.8)

These are extremal situations, which correspond to two totally different

topologies. In particular one could interpolate between these two antipodal situations and obtain intermediate situations, as shown in Figure 1.8.
It may be interesting to stress that every unitary matrix in U(4) determines a domain of self-adjointness for the operator in equation (1.19), which let us recover the topology of the classical configuration space Ω.
Using the Gel'fand - Naimark theorem [BR03] it is possible to retrieve from $D(H_U)$ the underlying topological space. Indeed, the space Ω and its topology can be recovered from the C^*-algebra generated by the continuos functions in $D(H_U)$.
One could even do more and try to recover the differentiable structure of Ω. For the interested reader we refer to [Bal+95].
The former construction can be generalized to higher dimensions. In particular, one could start with a couple of cylinders and check how topological configurations can be achieved by imposing different boundary conditions. For example we could have two separate cylinders, a single big torus or two disjoint tori. The allowed topology changes are much richer in this case, since one could even obtain an intermediate configuration of tori with holes. In this sense, a further generalization to surface with different genera can be done.
Indeed, by changing the corresponding unitary matrix one could obtain a manifold with genera $g_1 + g_2$ starting from manifolds with genera g_1 and g_2.
We would like to end this brief summary stressing the motivations for topology change in quantum gravity. So far we have discussed how to obtain topology change by means of external parameters, namely the unitary matrices which determine the self-adjoint extensions of the Hamiltonian operator. Indeed, these additional degrees of freedom can trigger a change in the boundary conditions, which reflect in the change of the topology of the underlying configuration space.
In [Bal+95] it is moreover discussed a resemblance of the previous mechanism with the axion approach to the strong CP problem in Quantum Chromodynamics [Pec08; Kim10]. In this case, in fact, the Hamiltonian operator describing the theory admits a one-parameter family of boundary conditions, namely U(1). The existence of these boundary conditions emerge in the term

$\theta \operatorname{Tr}(F \wedge F)$ which appears in the dynamical action. Moreover, if one let the boundary conditions change dynamically, then, the θ is promoted to an axion field, which represents an additional fluctuating degree of freedom.
In any case the introduction of additional degrees of freedom is responsible for a change in the topology of whatsoever configuration space we are considering.
Going back to quantum gravity, besides the spin-statistics connection there is also another motivation for the introduction of topology change. It has been speculated that Einstein's formulation of gravity represents only an effective model for a theory with additional degrees of freedom. Indeed, comparing and contrasting with other known models it has been suggested that ambiguities in the quantization procedure for gravity are due to an underlying structure and to its degrees of freedom. This ambiguity, for example, appears already in the Born-Oppenheimer approximation or in the two flavour Skyrme model and is solved by the introduction of an internal microstructure. In quantum gravity the eventual presence of geons highly complicates the situation and generates quantization ambiguities, which, from the experience accumulated from molecular and particle physics, may be overcome introducing new additional degrees of freedom, responsibile for a topology change.

1.3.1 Models of Topology Change

A rather recent paper [SWX12] has renewed interest in the topic, showing how unitary-preserving boundary conditions can be used to interpolate continuosly Hilbert spaces on different manifolds.
As already discussed in the previous section, topology changes are predicted in the realm of quantum gravity. As a matter of fact, it has been suggested that virtual processes may occur at very high energies causing an intense fluctuation in the space-time structure. Clearly this speculation is very far from being tested or even consistently supported by explict computations from quantum gravity.
Nevertheless, staying within the field of quantum mechanics, it has been suggested that, as discussed in the previous section, topology change may

occur varying some specific parameters appearing in the Hamiltonian, which encode the boundary conditions on the system.
In [SWX12] boundary conditions are implemented by means of projection operators, as we are going to show, and we are going to discuss how a fission of a mother interval into two daughter ones can be achieved, generating an entanglement entropy production. Let us consider a free quantum particle living on two separate half-lines, say, $(-\infty, a] \cup [b, \infty)$, described by the Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{1.28}$$

where m is the mass of the particle and $\hbar$ the Planck constant. From the Schrödinger equation we get the probability current, say

$$j = i\left(\psi^*\frac{\mathrm{d}}{\mathrm{d}x}\psi - \psi\frac{\mathrm{d}}{\mathrm{d}x}\psi^*\right). \tag{1.29}$$

If no probability flows out of the ends of the interval, then we have to impose that $j(a) = j(b) = 0$. Dirichlet, Neumann and Robin boundary conditions are just examples of boundary conditions satisfying the former constraint at the border. In particular, from a physical point of view, these are used to describe a quantum particle confined either in $(-\infty, a]$ or in $[b, \infty)$ with an initial probability of being in either one of them. This is not the full story. The conservation law, $\nabla \cdot j = 0$, allows a unitary dynamics through the border. For example the *identification* boundary conditions are allowed:

$$\begin{cases} \psi(a) = \psi(b) & , \\ \psi'(a) = \psi'(b) & , \end{cases} \tag{1.30}$$

where ψ' is the first derivative of ψ. In this case the two end points a and b can be identified, getting the quantum mechanical behaviour of a free particle on the real line. As already seen these two extreme situations can be encoded into a general framework, for example using unitary operators (in this case unitary matrices) at the boundary.
Alternatively one could use suitable projection operators, as we are going to discuss.

Let us denote by u the boundary data vector:

$$u = \begin{pmatrix} \psi(a) \\ \psi(b) \\ \psi'(a) \\ \psi'(b) \end{pmatrix}, \tag{1.31}$$

and consider the matrix:

$$J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{1.32}$$

Then, the continuity equation at the boundary can be written as: $u^\dagger J u = 0$. Suppose that u is a vector satisfying the previous equation, then it will encode some behaviour at the boundary. Indeed, boundary conditions can be implemented in terms of projections Π on the allowed vectors, say $u = \Pi\xi$, ξ being an arbitrary vector.
For example, Dirichlet boundary conditions are implemented by:

$$\Pi_D = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{1.33}$$

as it can be easily understood by a direct computation:

$$u = \begin{pmatrix} \psi(a) \\ \psi(b) \\ \psi'(a) \\ \psi'(b) \end{pmatrix} = \Pi_D \xi = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \xi_3 \\ \xi_4 \end{pmatrix}, \tag{1.34}$$

where $\xi_1, \xi_2, \xi_3, \xi_4 \in \mathbb{C}$. Similarly one can do for the *identification* boundary

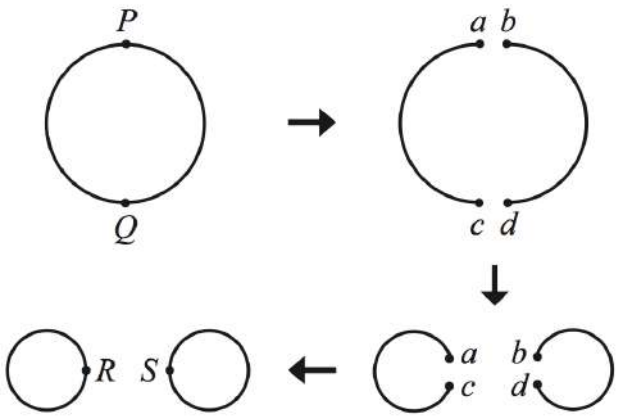

Figure 1.9: The pinching off of a *closed baby universe*. The circle on the left is broken in P and Q. Then the points a and c, b and d are joined together in the points R and S. Thus, two circles are obtained from one circle [SWX12].

conditions, say:

$$\Pi_{=} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \tag{1.35}$$

Thus the continuity equation can be recast as $\Pi^{\dagger} J \Pi = 0$, where Π is a two dimensional projection, since only two boundary conditions are needed.
With this technology at hand one can interpolate between different boundary conditions. For example, consider the following projection:

$$\Pi(\theta) = \frac{1}{2} \begin{pmatrix} c^2 & c^2 & cs & cs \\ c^2 & c^2 & cs & cs \\ cs & cs & 1+s^2 & -c^2 \\ cs & cs & -c^2 & 1+s^2 \end{pmatrix}, \tag{1.36}$$

where c stands for $\cos\theta$, s for $\sin\theta$ and $\theta \in (\pi, \pi)$. Manifestly one gets Dirichlet boundary conditions, for example for $\theta = \pi/2$, and the identification boundary conditions for $\theta = 0$.
We note that $\Pi(\theta)$ is a projection on the linear space spanned by the vectors $(0, 0, 1, -1)$ and (c, c, s, s). So, by continously passing from Π_D to $\Pi_{=}$ one

can describe a splitting operation, or, viceversa, by moving from $\Pi_=$ to Π_D a joining of the underlying topological space. These ideas can be be implemented to describe more complex topological changes, like the compression and the contraction of a closed early universe shaped like a circle (Figure 1.9), working with known quantum mechanical systems.
These ideas of interpolating between different topologies can be effectively extended to higher dimensions (Figure1.10). In higher dimensions technical details emerge on the role of the wavefunction and its normal derivative at the border (see Chapter 5).
Moreover, these surgery processes can generate entanglement. Consider, for the sake of simplicity, the process of fission of an interval $\Omega = [0, 2\pi]$ in two daughter intervals Ω_1 and Ω_2. Just like before we are going to consider a free particle described by the free Hamiltonian in equation (1.19). We are going to denote the mother interval's coordinates with $0 \leq x \leq 2\pi$ and the daughter's ones with $0 \leq y = x \leq \pi$ and $0 \leq z = 2\pi - x \leq \pi$. We are going to keep Dirichlet boundary conditions at $x = 0, 2\pi$ and $y = z = 0$ and adiabatically evolve from identification boundary conditions to Dirichlet in $x = y = z = \pi$. This midpoint fission of the mother interval induces a mapping between the respective Hilbert spaces and the corresponding bases:

$$L^2(0, 2\pi) \to L^2(0, \pi) \oplus L^2(0, \pi), \tag{1.37}$$

$$u_k = \frac{1}{\sqrt{2\pi}} \left(\sin kx + \sin \frac{2k-1}{2} x \right) \to \sqrt{\frac{2}{\pi}} \sin ky \oplus 0, \tag{1.38}$$

$$v_k = \frac{1}{\sqrt{2\pi}} \left(\sin kx - \sin \frac{2k-1}{2} x \right) \to 0 \oplus \sqrt{\frac{2}{\pi}} \sin kz, \tag{1.39}$$

where $k \in \mathbb{N}$. Then, if we start from the initial state $\sum_k (\alpha_k u_k + \beta_k v_k)$, an observer on the first daughter interval will have access to the reduced density matrix on its daughter interval, to which a non trivial von Neumann entropy is associated, namely:

$$S(\rho) = -\mathrm{Tr}(\rho \log \rho) = -r \log r - (1 - r) \log(1 - r), \tag{1.40}$$

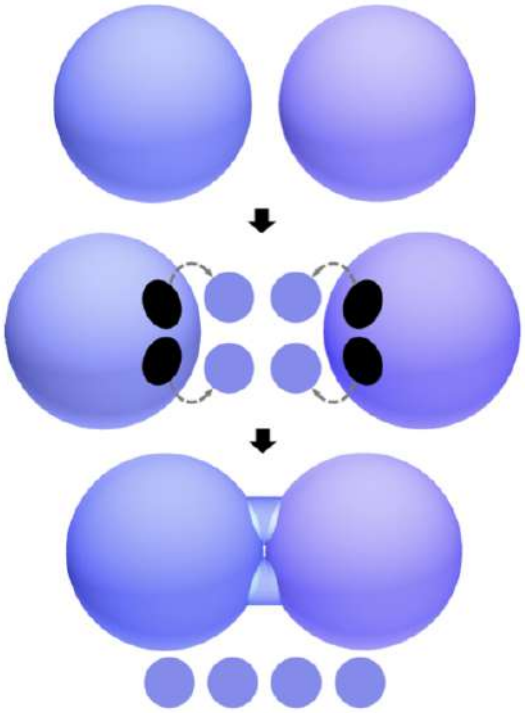

Figure 1.10: Continuous interpolation between quantum mechanics on two spheres and quantum mechanics on a torus plus four disks. This can be achieved with suitable boundary conditions [SWX12].

where $r = \sum_k |\beta_k|^2$. Moreover $S(\rho)$ is maximed when $\sum_k |\beta_k|^2 = \frac{1}{2}$.
This is not surprising since the von Neumann entropy represents the amount of intrinsical uncertainty of a quantum state. Indeed, when we restrict our attention and measurement processes to a singe interval we are depriving the observer of the information on what is happening on the other daughter interval.
From what has been discussed so far it is apparent how, even starting from a fission process on a single interval, one can have an increase in the entropy of a system due to a dynamical change in the topology.

1.4 The Quantum Hall Effect

In this section we are going to revise how boundary conditions emerge in the quantum Hall effect and what physical consequences they induce. First of all we are going to revise the classical version of this phenomenon.
The setup of the physical system is rather simple and it involves a two-dimensional gas of electrons under the influence of an intense magnetic field. The quantum Hall effect has proved to be useful in various areas of physics, e.g. in metrology, where it was used to determine with great accuracy the value of h/e^2 [KE85; Poi+11]. Not only solid state physics but basically every area of physics is connected to it. As a matter of fact the literature inherent to it is vast and it ranges from classical and quantum gravity [Myu99; Fab02; HOR04] to particle physics [Gre98; ZH01] and quantum computation [PVK98].

The classical Hall effect

The classical counterpart of this phenomenon was discovered by E. Hall in 1879, and it is a consequence of the motion of charged particles in a magnetic field. Consider a conducting strip on the $x-y$ plane (as shown in Figure 1.11) immersed in a uniform magnetic field B pointing in the z-direction. Suppose that a constant current flows in the x-direction. Then, if we measure the voltage at the ends of the strip (along the y-axis), we find a non zero value,

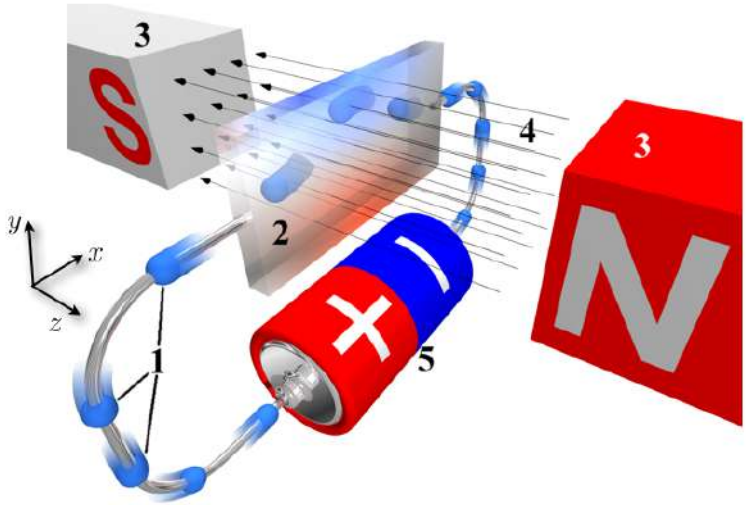

Figure 1.11: A flow of electrons (1) induced by the battery (5) passes through a metallic plate (2). A magnetic field (3) induced by a magnet (3) modifies the classical trajectories of the electrons, inducing a perpendicular voltage, known as the Hall voltage [Wik].

which is called the Hall voltage. This is the essence of the classical Hall effect.

Indeed, as known from elementary physics reasonings, charged particles are forced to move in circle under the action of a constant magnetic field at a constant frequency:

$$\omega_B = \frac{eB}{m}, \tag{1.41}$$

where e represents the electrical charge of the particles, while m their mass. The frequency ω_B is also known as the cyclotron frequency.

Using the Drude model and introducing an electric field E which accelerates the charges in its direction we can further generalize the Ohm law, namely: $J = \sigma E$, where J is the current density and σ the conductivity tensor:

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix}. \tag{1.42}$$

Thus, due to the introduction of a magnetic field the conductivity cannot

be a single number, but rather a matrix. From the Drude model [Jac98] it follows that:

$$\sigma = \frac{\sigma_{DC}}{1+\omega_B^2\tau^2}\begin{pmatrix} 1 & -\omega_B\tau \\ \omega_B\tau & 1 \end{pmatrix}, \qquad \sigma_{DC} = \frac{ne^2\tau}{m} \tag{1.43}$$

where τ is the scattering time, namely the average time between collisions of the electrons, and it is related to friction in the system due to the impurities of the material. Moreover, n is the density of the electrons, while σ_{DC} is the conductivity without a magnetic field. What really matters for the Hall effect are the anti-diagonal terms, which encode the information of a transversal current.

Indeed, the electrical current along the x-axis is deflected in the y-direction due to the magnetic field. This bending causes a charge separation between the edges which induces an electric field along the y-axis. The latter keeps on building up its intensity until the bending of the current along the x-axis is canceled. This induced electric field is responsible for the Hall voltage.

From an experimental point of view what is really measurable are the resistances, which can be calculated from the inverse conductivity matrix, say the resistivity:

$$\rho = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{yy} \end{pmatrix} = \sigma^{-1} = \frac{1}{\sigma_{DC}}\begin{pmatrix} 1 & \omega_B\tau \\ -\omega_B\tau & 1 \end{pmatrix} = \begin{pmatrix} \frac{m}{ne^2\tau} & \frac{B}{n\,e} \\ \frac{B}{n\,e} & \frac{m}{ne^2\tau} \end{pmatrix}. \tag{1.44}$$

Manifestly the off-diagonal terms are independent of τ meaning they capture some fundamental property of the material. Moreover, from the experimentalist's point of view one measures resistances, which depend on the geometry of the conductor, rather than resistivities.

In the Hall effect, the two quantities coincide. Indeed, consider a conductor of length L in the y-direction. If we apply a voltage V_y in the y-direction and measure the current I_x along the x-axis, we get for the transverse resistance:

$$R_{xy} = \frac{V_y}{I_x} = \frac{LE_y}{LJ_x} = -\rho_{xy}. \tag{1.45}$$

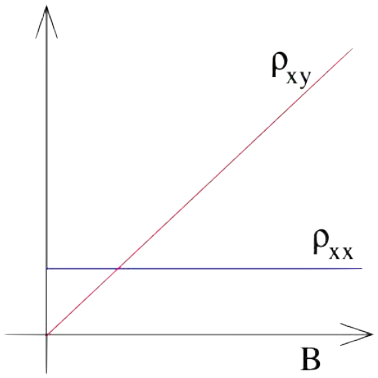

Figure 1.12: Prediction of ρ_{xy} and ρ_{xx} in the classical Drude model

The situation for R_{xx} is completely different, since, in that case the respective lengths involved will not cancel out.
Eventually, the Drude model makes experimental predictions for the resistivities (Figure 1.12), namely :

$$\rho_{xx} = \frac{m}{n\, e^2\, \tau}, \tag{1.46}$$

$$\rho_{xy} = \frac{B}{n\, e}. \tag{1.47}$$

The quantum Hall effect

As history testifies, the former predictions were falsified under certain conditions. For this part of the story we highly recommend [Kli05].
In 1980 K. von Klitzing [KDP80] discovered, due to quantum behaviours, new fascinating aspects in the Hall effect. The experiment was conducted on a MOSFET at low temperatures (namely 4.2 K) in order to suppress disturbing scattering processes and at very intense magnetic fields. The use of strong magnetic fields had already been employed in order to investigate the inner structure of semiconductors.
Interestingly, the transversal resistivity, that is ρ_{xy}, does not have a linear behaviour as predicted by the classical model but it rather shows regular jumps and large plateaus (Figure 1.13). Moreover, ρ_{xx} is almost everywhere zero but in correspondence of the jumps. From the analysis of the experimental

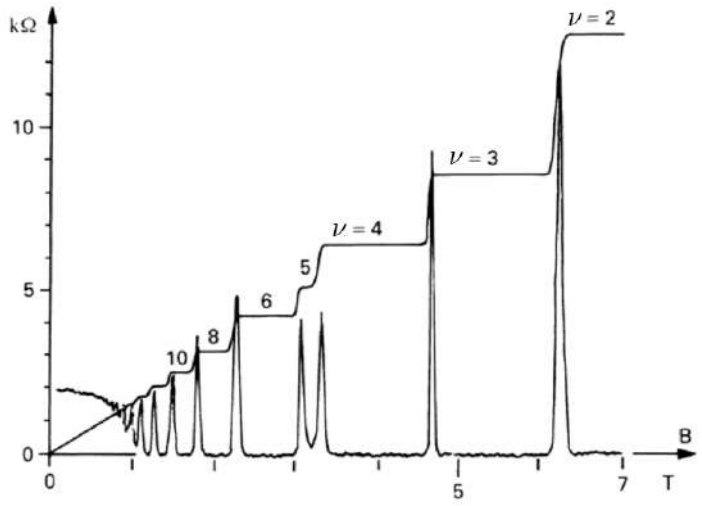

Figure 1.13: The integer quantum Hall effect. The Hall resistance changes stepwise when the magnetic field B varies. Every step is indexed by an integer ν, such that its height is inversely proportional to it. The lower curves with peaks at every steps represents the Ohmic resistance[Sci].

data it was shown that:

$$\rho_{xy} = \frac{2\pi\hbar}{e^2\nu} \qquad , \qquad \nu \in \mathbb{N}. \tag{1.48}$$

The plateaus bring no additional information neither on the charge density nor on the magnetic field nor on the geometrical structure of the device. The measurement was so precise that the quantum of resistivity, that is $2\pi\hbar/e^2$ is used as a standard in the measure of resistivity, for this effect is highly stable and easily reproducible.

The integer nature of the resistivity can be explained in terms of the energy spectrum of the electron gas [Lau81]. Indeed, electrons can accumulate on a surface of a single crystal by an applied positive voltage at the gate and consequently form a two-dimensional gas [Fow+66]. Even in the approximation of non interacting electrons, the energy of the free electrons is quantized under an intense magnetic field. This is nothing but Landau quantization of

energy levels for the Hamiltonian:

$$H = \frac{1}{2m}\left(p_x^2 + (p_y + eBx)^2\right), \tag{1.49}$$

in the Landau gauge [LL77]. The highly degenerate discrete spectrum reads:

$$E_\nu = \hbar\omega_B\left(\nu + \frac{1}{2}\right) \quad , \qquad \nu \in \mathbb{N}. \tag{1.50}$$

The former energy levels have gaps within and it is exactly when the Fermi energy crosses one of the gaps that the quantum Hall effect comes on stage. Of course, since the temperature is kept extremely low, then, excitations across the gaps are not allowed.
From this explanation it follows that $\rho_{xy} = 2\pi\hbar/e^2\nu$ happens exactly when ν Landau levels are filled.

Edge modes and quantum boundary conditions

Another interesting fact happens at the border of the system, with the existence of the so called *edge modes*. Electrons, and more generally charged particles, tend to rotate in one and only one direction in a uniform magnetic field. But what happens when they collide with the border? From a classical point of view they are forced to bounce back and reflect in order to keep on rotating in the direction forced by the magnetic field. Then, we observe an overall skipping motion where the particles along one side of the boundary move in a single and well determined direction.
For this reason every edge can carry a current, called a *chiral current* because electrons are forced to move in one direction determined by the relative orientation of the magnetic field and the edge, even in equilibrium. These effects were largely studied in [Hal82; Tho93; Mac90; Wen90; Wen91; Wen92; MF94].
These states are very robust because there is a large energy gap between the Fermi energy and the energy associated to states in the bulk. For this reason disorder cannot mix edge states with states in the bulk so that some current may escape from the edge region. In addition to that, chirality plays

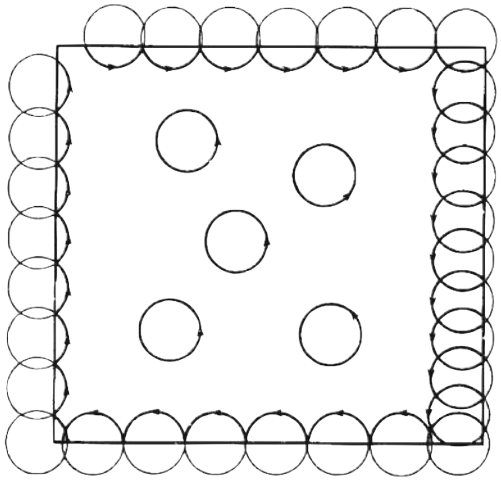

Figure 1.14: In this picture electrons in the bulk rotate anticlockwise. Electrons near the boundary scatters at the edge, determining an overall clockwise current [Pei79].

a fundamental role as well. Indeed, it prevents electrons from backscattering at the edge even when disorder comes on stage. For these reasons the Hall currents and the quantum version of the Hall effect are very robust as long as the Fermi energy level lies in the gap between Landau levels in the bulk [Hal82].

Moreover it has been largely investigated the connection between the physics of the quantum Hall effect and the boundary conditions to be imposed at the edges of the sample [QT87; IMT96; Akk+98].

Indeed there are mainly two directions while investigating the quantum Hall effect: on the one hand one could be interested in the two dimensional characteristics of the system which emerge in the bulk, on the other one could be concerned about the one dimensional boundary effects. The chirality at the edge plays a fundamental role in the choice of suitable boundary conditions [Akk+98]. As already remarked, from a classical point of view, moving electrons in a magnetic field are forced on circular trajectories.

In particular, if the electrons in the bulk rotate clockwise, then, the net current at the boundary flows anti clockwise due to the skipping orbits of electrons close to the edges [RB85] (see Figure 1.14).

It is plain to see that, already classically, bulk and edge are distinguished by the chirality relative to the boundaries. This distinction can be achieved quantum mechanically with the aid of suitable boundary conditions to be imposed on the Hamiltonian. The chiral boundary conditions are highly dependent on the direction of the tangential velocity at the border.
In particular the Hilbert space splits into a direct sum of Hilbert spaces with positive and negative chiralities. Consequently, under the action of a magnetic field, the total Hilbert space splits in a Hilbert space for edge states, say $\mathcal{H}_e$ and one for bulk states, namely $\mathcal{H}_b$, so that the full Hilbert space reads $\mathcal{H} = \mathcal{H}_e \oplus \mathcal{H}_b$. This splitting causes a separation in the spectrum for the bulk and the edge component.
Interestingly, under chiral boundary conditions the bulk spectrum has a ground state which corresponds to the lowest Landau level for a gas of non-interacting electrons in an infinite plane and it is highly degenerate. The degree of degeneracy consists in the total flux of the magnetic field through the gas.
The edge spectrum, instead, is always discrete for any boundary with finite length and, in the thermodynamic limit of long boundary, gets gapless.
For this model one considers a semi-infinite cylinder M (See Figure 1.15), where chiral boundary conditions will be imposed. In particular the boundary of M, say ∂M is a circumference of length l, so that M reads:

$$M = \{(x, y) \in \mathbb{R}^2 \,|\, x \leq 0\,,\, 0 \leq y \leq l\}. \tag{1.51}$$

Moreover M is an oriented surface, that is, we suppose that M keeps always on the left while walking around the border of M. We suppose that a constant magnetic field $B > 0$ is perpendicular to the surface. We will also a have a longitudinal magnetic field such that its flux tube ϕ passes through the cylinder. In this analysis the magnetic field B will play the role of a fixed constant, while, ϕ a changing parameter.
A suitable vector potential describing this situation is:

$$A = \left(0, B\,x + \frac{\phi}{l}\right). \tag{1.52}$$

For simplicity in the notation we are going to settle $m = \hbar = e/c = 1$, where m is the mass of the electron, e its electrical charge and c the speed of light. With this convention the velocity operator reads:

$$(v_x, v_y) = \left(-i\frac{\partial}{\partial x}\,,\, -i\frac{\partial}{\partial y} - Bx - \frac{\phi}{l} \right), \tag{1.53}$$

so that the Landau Hamiltonian is given by:

$$H_L(\phi) = \frac{1}{2} D^\dagger(\phi) D(\phi) + \frac{B}{2}, \tag{1.54}$$

where,

$$D(\phi) = iv_x - v_y = \frac{\partial}{\partial x} + \left(i\frac{\partial}{\partial y} + Bx + \frac{\phi}{l} \right). \tag{1.55}$$

Clearly this is only a formal expression for the Landau Hamiltonian, in order to make it self-adjoint we need to impose boundary conditions on ∂M. These boundary conditions will implement the chiral behaviour of the current at the edges. Since $v_y(\phi, 0) = -i\partial_y - \phi/l$ commutes with D we separate variables and describe the chiral boundary conditions for the resulting ordinary differential operators on the half-line, parametrized by $m \in \mathbb{Z}$ and $\phi \in \mathbb{R}$:

$$H_L(\phi) = \bigoplus_{m \in \mathbb{Z}} H_m(\phi), \tag{1.56}$$

$$2H_m(\phi) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \left(\frac{2\pi m - \phi}{l} - Bx \right). \tag{1.57}$$

If we define

$$D_m(\phi) = \frac{\mathrm{d}}{\mathrm{d}x} - \frac{2\pi m - \phi}{l} + Bx, \tag{1.58}$$

then the chiral boundary conditions can be written as:

$$\begin{cases} (D_m\psi)(0) = 0, & \text{if} \quad v_y(\phi, 0) = \frac{2\pi m - \phi}{l} \leq 0, \\ iv_x\psi(0) = 0, & \text{if} \quad v_y(\phi, 0) = \frac{2\pi m - \phi}{l} > 0. \end{cases} \tag{1.59}$$

Classically an electron in the bulk rotates clockwise, so that its velocity near the boundary does not agree with the orientation of the boundary itself. For

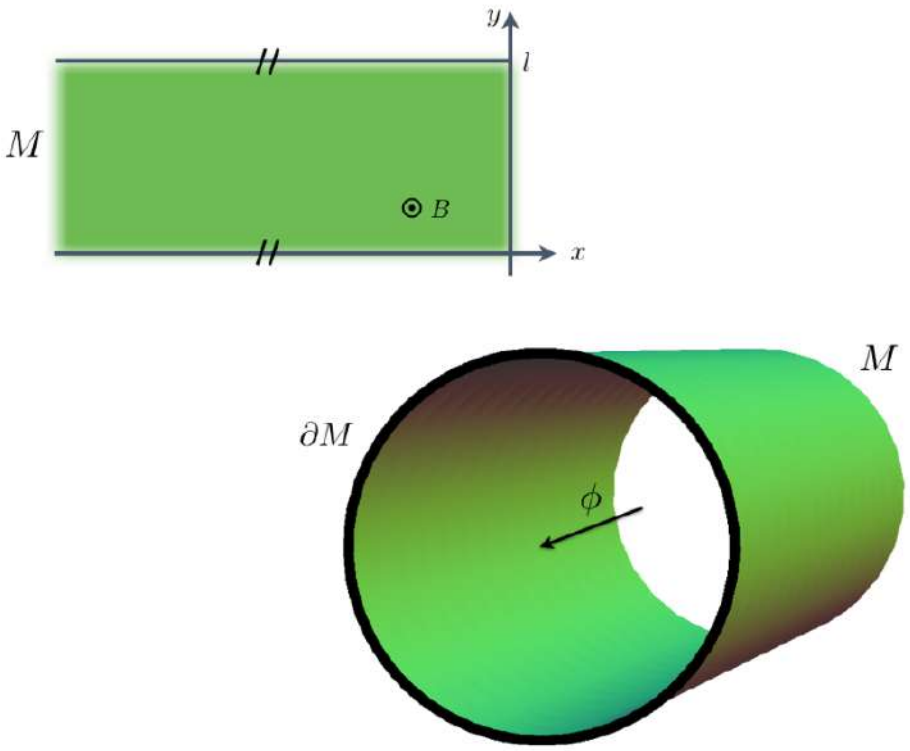

Figure 1.15: Here represented the semi-cylinder described in equation (1.51). On the upper-left part the unrolled cylinder is shown, with opposite side identified. We recall that the magnetic field B is orthogonal to the surface, while the fixed flux ϕ passes through the cylinder.

these electrons the first kind of boundary conditions are imposed, that is $(D_m\psi)(0) = 0$. These boundary conditions, called *spectral boundary conditions*, depend on m and they represent an interpolation between Neumann and Dirichlet boundary conditions.
On the contrary a skipping particle agrees with the orientation of M. For this reason Neumann boundary conditions are imposed for positive velocities. The Hamiltonian in equation (1.57) with the boundary conditions given by (1.59) is self-adjoint.
Moreover the bulk Hilbert space is generated by the family $\{e^{2\pi imy/l} f_m(x)\}$, where f_m are the eigenfuctions of the Hamiltonian with spectral boundary conditions. The edge Hilbert space, instead, is its orthogonal complement.
As expected, the spectrum of this operator depends on the boundary conditions chosen. Indeed, the energy of the ground state for the bulk reads $B/2$, which corresponds to the lowest Landau energy level in the plane and the degeneracy equals the total magnetic flux.
In addition to that, the edge spectrum is purely discrete for any finite boundary length l. In the thermodynamic limit the edge spectrum gets gapless and one can associate from the curves appearing in the spectrum a linear dispersion law. For this reason there is a unique sound velocity associated to the chiral edge currents, which reads $\sqrt{B/\pi}$.
Playing with the boundary conditions, then one can obtain different physical consequences. Dirichlet boundary conditions, $\psi(0) = 0$, generate an explicitly solvable spectral problem. Nevertheless there is no net separation between the bulk and the edge, no unique velocity for the edge currents and no macroscopic degeneracy appears for the ground state.
An interesting comparison can be made with APS (Atiyah-Patodi-Singer) boundary conditions [APS75] which read:

$$\begin{cases} (D_m\psi)(0) = 0, & \text{if} \quad v_y(\phi, 0) = \frac{2\pi m - \phi}{l} \leq 0, \\ \psi(0) = 0, & \text{if} \quad v_y(\phi, 0) = \frac{2\pi m - \phi}{l} > 0. \end{cases} \tag{1.60}$$

For these boundary conditions states with different chirality are sharply separated, as expected. However the edge states have a small density near the

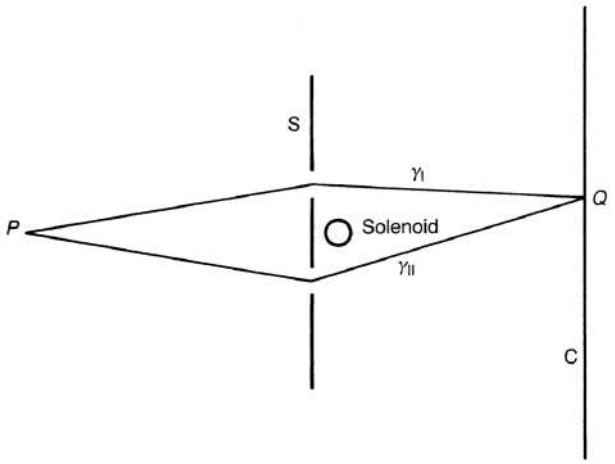

Figure 1.16: A schematic illustration of the Aharonov-Bohm experimental setup.

boundary and tend to be pushed away from the boundary. This goes strongly against the robustness of the quantum Hall effect.
Interestingly, the chiral boundary conditions are linked to the Laughlin states, which were introduced by Laughlin [Lau83] in order to explain the fractional quantum Hall effect. We refer the interested reader to [Eze08].

1.5 The Aharonov-Bohm effect

Another interesting phenomenon where the boundary conditions play a fundamental role is the Aharonov-Bohm effect [AB59].
In this quantum-mechanical effect a charged particle is influenced by an electromagnetic potential although it is confined in a region with no electric or magnetic field. This has no classical explanation since what really matters at the level of the classical equations of motion are the magnetic and electric fields generated by those potentials. For this reason, the motion of a classical charged particle is unaffected in a region where the magnetic field is zero, although the vector potential $\boldsymbol{A}$ is not.
From a quantum mechanical point of view, instead, there is a coupling between the complex phase associated to the wave function of a charged particle

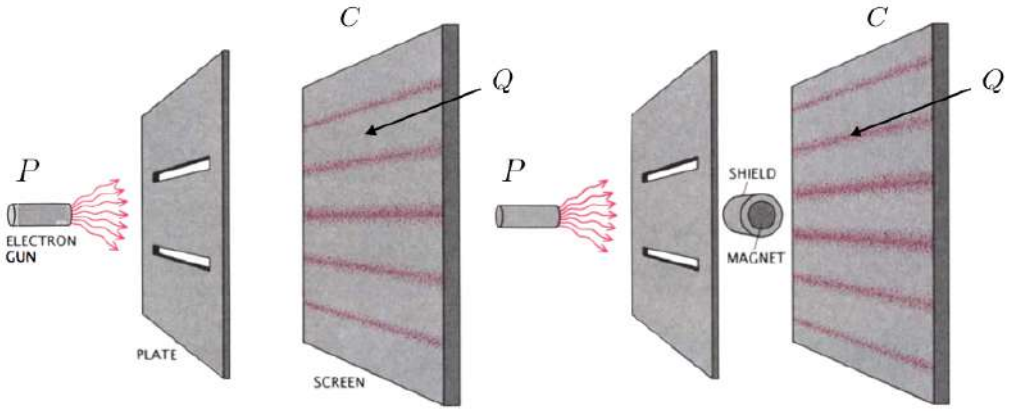

Figure 1.17: A shift of the electrons' interference pattern due to the vector potential associated to the magnetic field threading the solenoid.

and the electromagnetic potential, rather than the associated fields [Dir31a]. So that, even if a charged particle passes through a region where there is no magnetic field, then the phase associated to its wave function gets affected. The existence of this phase can be demonstrated by means of interference experiments.

We are going to briefly recall the experimental setup. The Aharonov-Bohm experiment is schematically illustrated in Figure 1.16. An electron source is placed at the point P, while in the middle a double slit with a solenoid sits next to it. In the point C, instead, there is a screen to observe interference patterns. The solenoid is shielded so that no electrons can penetrate it. We suppose that the radius of the solenoid is infinitesimally small.

If one keeps the total magnetic flux fixed, say $\Phi = \int_S \boldsymbol{B} \cdot \mathrm{d}\vec{S}$, S being the section of the solenoid, then one can choose the electromagnetic potentials in this form:

$$\boldsymbol{A} = \left(-\frac{y\,\Phi}{2\pi r^2}, \frac{x\,\Phi}{2\pi r^2}, 0 \right) \quad , \qquad A_0 = 0 \tag{1.61}$$

so that $\int_S \nabla \times \boldsymbol{A} = \Phi$ and $\boldsymbol{B} = \nabla \times \boldsymbol{A} = 0$ outside the solenoid. In this configuration the vector potential does not vanish outside the solenoid while the magnetic field does. From a classical point of view, as already stressed, the magnetic field generated by the solenoid cannot influence the motion of

the electrons because the Lorentz force vanishes on the path of the beam. Instead, from a quantum mechanical point of view, it generates a shift in the interference pattern. Indeed, a wave function in a spatial region where there is a non zero vector potential $\boldsymbol{A}$ reads:

$$\psi = \psi_0 \, \mathrm{e}^{\frac{ie}{\hbar c} \int \boldsymbol{A}(\vec{x}) \mathrm{d}\vec{x}}, \tag{1.62}$$

where ψ_0 is the wave function with zero vector potential and the integral is taken along a path starting in P and ending in the point we are interested in, for example the point Q on the screen.
In order to determine the interference pattern in Q, one considers the superposition:

$$\Psi = \psi_1 + \psi_2 = \psi_{1,0} \, \mathrm{e}^{\frac{ie}{\hbar c} \int_{\gamma_1} \boldsymbol{A}(\vec{x}) \mathrm{d}\vec{x}} + \psi_{2,0} \, \mathrm{e}^{\frac{ie}{\hbar c} \int_{\gamma_2} \boldsymbol{A}(\vec{x}) \mathrm{d}\vec{x}}, \tag{1.63}$$

which can be proved to equal:

$$\Psi = \left(\psi_{1,0} \, \mathrm{e}^{\frac{ie}{\hbar c} \Phi} + \psi_{2,0} \right) \mathrm{e}^{\frac{ie}{\hbar c} \int_{\gamma_2} \boldsymbol{A}(\vec{x}) \mathrm{d}\vec{x}}, \tag{1.64}$$

where Φ, is the solenoid flux defined above. Then, the interference pattern reads:

$$|\Psi|^2 = |\psi_{1,0}|^2 + |\psi_{2,0}|^2 + 2 \, \mathrm{Re} \left(\psi_{1,0}^* \psi_{2,0} \, \mathrm{e}^{-\frac{ie}{\hbar c} \Phi} \right). \tag{1.65}$$

Evidently, one can observe a shift in the usual interference pattern due to the presence of the solenoid, which appears in the term with the magnetic flux Φ.
The effect was first experimentally checked in 1960 [Cha31] using an experimental apparatus similar to the one described above. Then, it was confirmed in 1962 [MB62] and later on under several different configurations using optical and electron holography [Ta82] and toroidal permalloy [Ta86]. More recently, instead, the Aharonov-Bohm effect was tested in quantum interference devices [NB09] and graphene rings [Sa86].
The solenoid in the Aharonov-Bohm effect induces a perturbation in the

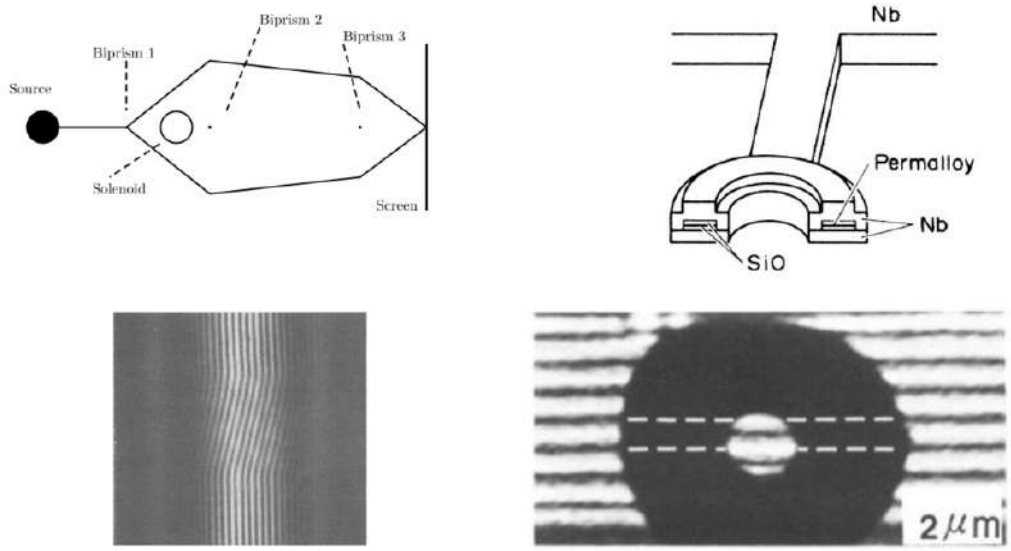

Figure 1.18: Experimental evidence of the Aharonov-Bohm effect. On the left interference pattern with fringe shifts [MB62]. On the right the experimental setup by Tonomura et al. [Ta86]. In this case the dashed lines make the electrons' shift visible.

configuration space crossed by the electrons, which can be encoded by means of boundary conditions. In order to discuss the role of boundary conditions for the Aharonov-Bohm effect see [OP10].

The objective here is to characterize all the possible boundary conditions on the border S of the solenoid consistent with the structure of quantum mechanics. Moreover we are going to deal with regular realizations, whose domains are subspaces of $H^2(S')$, where $S' = \mathbb{R}^2 \setminus S$ is the region outside the solenoid and $H^2(S')$ is the second Sobolev space on S'.

As in the previous discussion we suppose that the solenoid, of radius a, is centered at the origin of the x-y plane, with its axis on the z direction. We suppose that a stationary current through it generates a uniform magnetic field confined in the interior of the solenoid. We suppose that a spinless particle with mass $m = 1/2$ can move in S' and cannot interact with the magnetic field. Denoting with $\boldsymbol{A}$ the vector potential associated with the magnetic field and setting $\hbar = 1$, then the Hamiltonian for the charged

particle reads:

$$H = \left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 \qquad \boldsymbol{p} = -i\,\nabla \tag{1.66}$$

where e is the electric charge, c the speed of light, and the domain of the Hamiltonian reads $D(H) = C_0^\infty(S')$, the space of regular functions with compact support in S'.

This operator is not self-adjoint but solely symmetric [OP10]. Indeed, as long as we do not take into account the interaction of the charged particles with the boundary then, the Hamiltonian operator cannot describe a physical observable. Indeed, the space $C_0^\infty(S')$ does not contain information of the interaction of the wave functions with the solenoid.

Usually Dirichlet boundary conditions are imposed on the solenoid [OP08]. Nevertheless, this is not the full story because there may be different interactions between the particles and the solenoid. These different interactions can be encoded in different boundary conditions, as we are going to discuss. Indeed, it will be important to select those boundary conditions that describe a particle moving in S' and which cannot penetrate the solenoid, but can only interact with its boundary. From a quantum mechanical point of view, we need to select the boundary conditions which realize self-adjoint realizations of the Aharonov-Bohm Hamiltonian, and which reproduce this interaction with different interface materials.

Let us consider the vector potential $\boldsymbol{A}$ in polar coordinates (r, θ) in the plane, such that:

$$\boldsymbol{A} = (A_r, A_\theta) \qquad A_r = 0 \qquad A_\theta = \frac{\Phi}{2\pi r}, \tag{1.67}$$

for $r \geq a$ and where Φ is the total magnetic flux through the solenoid. This symmetric operator admits self adjoint realizations since its deficiency indices are both equal and infinite [RS75].

Moreover we are not going to deal with every possible self-adjoint extension, rather we will mainly interested in those whose domains are subspaces of $H^2(S')$. Due to the symmetry of the system we are going to consider planar sections of the solenoid.

As discussed in section 1.3 the lack of self-adjointness of a symmetric operator

is directly linked to the boundary form associated with it, namely:

$$\Gamma(\psi,\phi) = \langle \psi, H^*\phi\rangle - \langle H^*\psi, \phi\rangle, \tag{1.68}$$

for all ψ and $\phi \in D(H^*)$. Passing to polar coordinates (r,θ), the boundary form reads:

$$\begin{aligned}\Gamma(\psi,\phi) &= a\int_0^{2\pi} \mathrm{d}\theta \Bigg(\overline{\frac{\partial\psi}{\partial r}(a,\theta)}\phi(a,\theta) - \overline{\psi(a,\theta)}\frac{\partial\phi}{\partial r}(a,\theta) \\ &+ 2i\overline{\psi(a,\theta)}(\boldsymbol{A}\cdot\mathbf{r})\phi(a,\theta)\Bigg).\end{aligned} \tag{1.69}$$

It can be proved with the technique of the boundary triples [BGP08] that all the self-adjoint realizations of the Aharonov-Bohm Hamiltonian in $H^2(S')$ are parametrized uniquely by unitary operators on $L^2(S)$, namely

$$H_U\psi = H^*\psi \qquad \psi \in D(H_U), \tag{1.70}$$

$$D(H_U) = \left\{ \psi \in H^2(S') \,:\, i(I+U)\psi(a,\theta) = (I-U)\frac{\partial\psi}{\partial r}(a,\theta) \right\}. \tag{1.71}$$

For example:

- If $U = I$, then we get Dirichlet boundary conditions:

$$D(H_U) = \left\{\psi \in H^2(S') \,:\, \psi(a,\theta) = 0\right\} = H^2(S') \cap H_0^1(S'). \tag{1.72}$$

  These boundary conditions have already proved their usefulness in the physical description of the phenomenon [OP08; Rui83].

- If $U = -I$, then we get Neumann boundary conditions:

$$D(H_U) = \left\{ \psi \in H^2(S') \,:\, \frac{\partial\psi}{\partial r}(a,\theta) = 0 \right\}. \tag{1.73}$$

- $U = -\exp(-i\,u(\theta))$, where u is a measurable function on S. If $1+U$ is

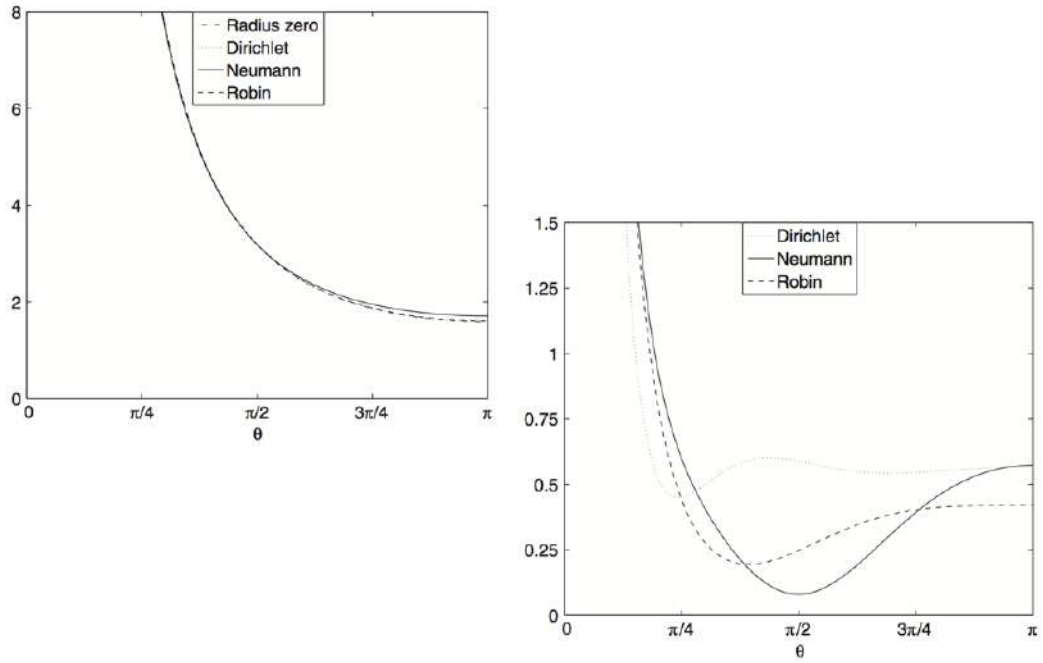

Figure 1.19: A comparison between different scattering sections with different boundary conditions [OP10].

invertible, or equivalently if the function

$$f(\theta) = i\frac{\mathrm{e}^{i\,u(\theta)} - 1}{\mathrm{e}^{i\,u(\theta)} + 1} \tag{1.74}$$

is well defined, real and measurable, then the corresponding extension reads:

$$D(H_U) = \left\{ \psi \in H^2(S') \,:\, \frac{\partial \psi}{\partial r}(a,\theta) = f(\theta)\psi(a,\theta) \right\}. \tag{1.75}$$

These are nothing but Robin boundary conditions.

Up to now we have discussed the case of a solenoid with a finite radius, say $a > 0$ and the regular self-adjoint realizations of the system.
With these results at hand one can study scattering processes with different boundary conditions. For example the case of Dirichlet boundary conditions was investigated in [Rui83].

More generally, different boundary conditions generate different scattering cross sections, which can be experimentally measured. With this idea in mind, then, one could understand which kind of interaction can occur between the electrons and the wall, because mostly it is not clear what boundary conditions are realized in laboratories.
Figure 1.19 shows qualitatively what was mentioned. On the left it is represented the low-energy behaviour of the differential cross sections obtained with different boundary conditions. In this case they almost behave the same way, so it is not possible to tell which boundary conditions have contributed the most. Differently, on the right the same differential cross sections are plotted at higher energy. Interestingly enough there is a sharp separation between them, so that different boundary conditions can be experimentally told apart. For a further discussion of the different cross sections and their comparison we refer the reader to the aforementioned paper [OP10].
These results can be compared with the ones in [AT98; DS98], where the radius of the solenoid is shrinked to 0. In this case the deficiency indices are equal to 2 and the self-adjoint realizations are parametrized in terms of 2×2 unitary matrices. Scattering cross sections in the presence of zero radius solenoids are also discussed in [AT98; AB59; DS98; Hag90; PR11].
Other interesting results on the interplay between boundary conditions and the Aharonov-Bohm effect can be found in [ESV02], where all the admissible boundary conditions are determined and classified and in [GER09], where the role of the charge transport at the edge of a Hall system in terms of heat is analyzed.

1.6 Why self-adjointness? The global theory of quantum boundary conditions.

Up to this point we have made a large use of words like *self-adjointness* and *quantum boundary conditions*, stressing their physical relevance without entering too much into details.
In Chapter 5 we are going to deal with all the rigorous details and results

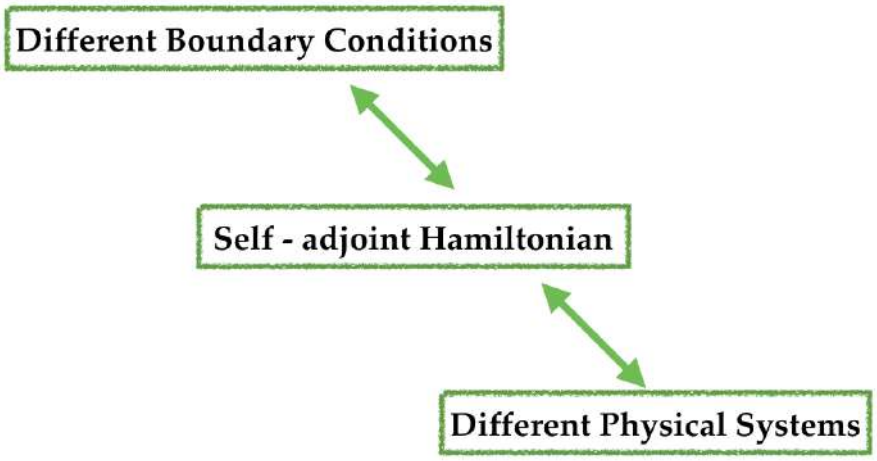

Figure 1.20: Why self-adjointness?

which have been hidden under the carpet so far.
For now, we would only give a brief introduction about the connection which resides between self-adjoint operators and quantum boundary conditions.
In particular, it is well known that in quantum mechanics the physical observables are represented by self-adjoint operators, mainly for two reasons. The first one is kinematical and resides in the spectral theorem.
By the spectral theorem [RS75] it is well known that every self-adjoint operator H admits a unique decomposition in terms of projection valued measures, $\Omega \mapsto P_H(\Omega)$, and its spectrum is real:

$$H = \int_{\mathbb{R}} \lambda \, \mathrm{d}P_H(\lambda). \tag{1.76}$$

The spectrum of a self-adjoint operator is, for this reason, linked to the measurable values of the associated observable.
Self-adjoint operators are also necessary from a dynamical point of view. As a matter of fact, Stone's theorem [RS75] estabilishes a one-to-one correspondence between (strongly continuous) one-parameter unitary groups and self-adjoint operators. For this reason self-adjoint operators are interpreted as the infinitesimal generators of the admissible transformations on the Hilbert space of physical states.
In particular, the dynamics of a closed quantum system is governed by a

unitary group V, whose generator is the Hamiltonian operator H:

$$V(t) = \mathrm{e}^{-\frac{i\,t}{\hbar}H} \qquad , \qquad t \in \mathbb{R}. \tag{1.77}$$

Usually, the starting point is looking for an operator which could be a good candidate for representing an observable. Then, one starts searching for some symmetric domain of definition and tries to check whether the closure of the respective operator is self-adjoint. In the negative case one is forced to study various (if any) self-adjoint extensions of the operator under examination.
Interestingly, for some operators the self-adjoint extensions can be parametrized in terms of boundary conditions. Moreover, different boundary conditions for the same Hamiltonian operator correspond to distinct physical systems since they exhibit different spectra and dynamics.
Indeed, from the axioms of Quantum Mechanics, it is well known that the spectrum of a self-adjoint operator representing an observable is linked to its measurable values.
Here we briefly recall some of the main results used up to this point in order to characterize the physical realizations of the Hamiltonian in terms of boundary conditions.
For the sake of concreteness we will discuss only the one-dimensional case [AIM05]. For further generalization we refer to Chapter 5.
Consider a free quantum particle confined in a one dimensional segment $\Omega = (0, 1)$. This situation is effectively described in the Hilbert space $L^2(\Omega)$ by the Hamiltonian operator:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{1.78}$$

where m is the mass of the particle and $\hbar$ the Planck constant. This operator is solely symmetric on $D(H) = C_0^\infty(0, 1)$ and, as such, it cannot represent a physical observable. Nevertheless it is a good candidate and, for this reason, one looks for its self-adjoint extensions.
We recall that the adjoint of H, say H^*, acts as in equation (1.78) in the distributional sense on a larger domain, that is $D(H^*) = H^2(\Omega)$, the space of

square integrable functions whose first and second distributional derivative are square integrable as well. In particular, every self-adjoint realization will be obtained as a restriction of $D(H^*)$ with certain boundary conditions:

$$D(H^*) \cap \{\text{suitable boundary conditions}\}. \tag{1.79}$$

First of all, making use of von Neumann's theory, one can prove that H admits self-adjoint extensions because its deficiency indices are equal [Neu55]. Then, it can be proved [AIM05] that the set of self-adjoint extensions of H is in one -to -one correspondence with the group of 2×2 unitary matrices. Namely every physical realization of H, say H_U is given by a unitary matrix U, such that its domain reads:

$$D(H_U) = \{\psi \in H^2(\Omega) : \ \mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}\},$$

where φ and $\dot{\varphi}$ are the boundary data of the wave function ψ and are defined as

$$\varphi := \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix}, \qquad \dot{\varphi} := \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix}. \tag{1.80}$$

where the minus signs, which appears in the $\dot{\varphi}$ vector, is chosen such that the normal vector field on the boundary $\partial\Omega = \{0, 1\}$ points outward. Choosing different unitary matrices one obtains distinct boundary conditions: For example:

$$U = \mathbb{I}, \qquad \psi(0) = 0 = \psi(1), \qquad \text{Dirichlet;} \tag{1.81}$$

$$U = -\mathbb{I}, \qquad \psi'(0) = 0 = \psi'(1), \qquad \text{Neumann;} \tag{1.82}$$

$$U = -\sigma_1, \qquad \psi(0) = \psi(1)\,,\ \psi'(0) = \psi'(1), \qquad \text{periodic;} \tag{1.83}$$

$$U = \sigma_1, \qquad \psi(0) = -\psi(1)\,,\ \psi'(0) = -\psi'(1), \qquad \text{antiperiodic.} \tag{1.84}$$

where σ_1 is the first Pauli matrix. Dirichlet and Neumann boundary conditions are particular cases of local boundary conditions. The respective unitary matrices are diagonal and they do not mix the boundary values at the border. The nondiagonal ones, like $U = \sigma_1$, describe nonlocal boundary

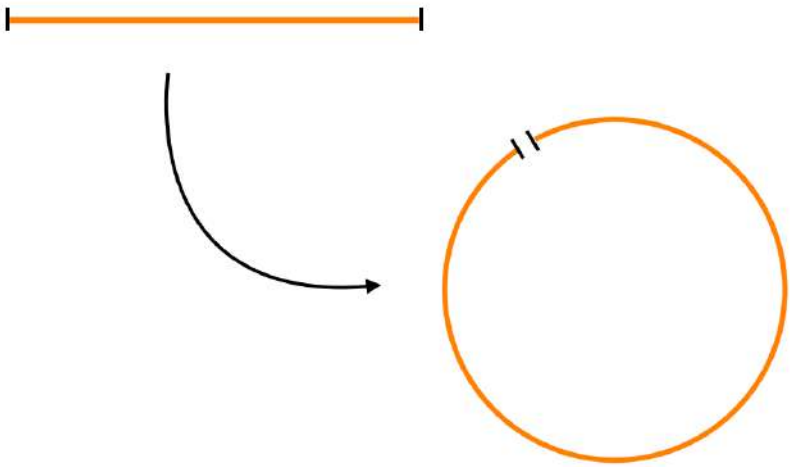

Figure 1.21: A change in the topology induced by non diagonal unitary matrices.

conditions, which mix the values at the border.
In order to preserve unitarity, or in other words "what comes out from one end of the interval must return to the other one", we need to bend the interval so that the interval endpoints become the two sides of a junction. Thus, passing from a diagonal U to a non diagonal one, we are changing the underlying topology from an interval to a circle (see Figure 1.21 and Figure 1.22). If the junction is impermeable, the walls are completely reflecting, otherwise there could be some probability flux across the junction, from one wall to the other. For example, consider the matrix

$$U = -\begin{pmatrix} 0 & \mathrm{e}^{-\mathrm{i}\alpha} \\ \mathrm{e}^{\mathrm{i}\alpha} & 0 \end{pmatrix}, \tag{1.85}$$

which describes pseudo-periodic boundary conditions:

$$\psi(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi(0), \qquad \psi'(1) = \mathrm{e}^{\mathrm{i}\alpha}\psi'(0). \tag{1.86}$$

When passing through the junction, the wave function acquires a phase α. If $\alpha = 0$ we return to periodic boundary conditions, and the underlying topology is the one of a circle. Otherwise, if $\alpha = \pi$ we get antiperiodic

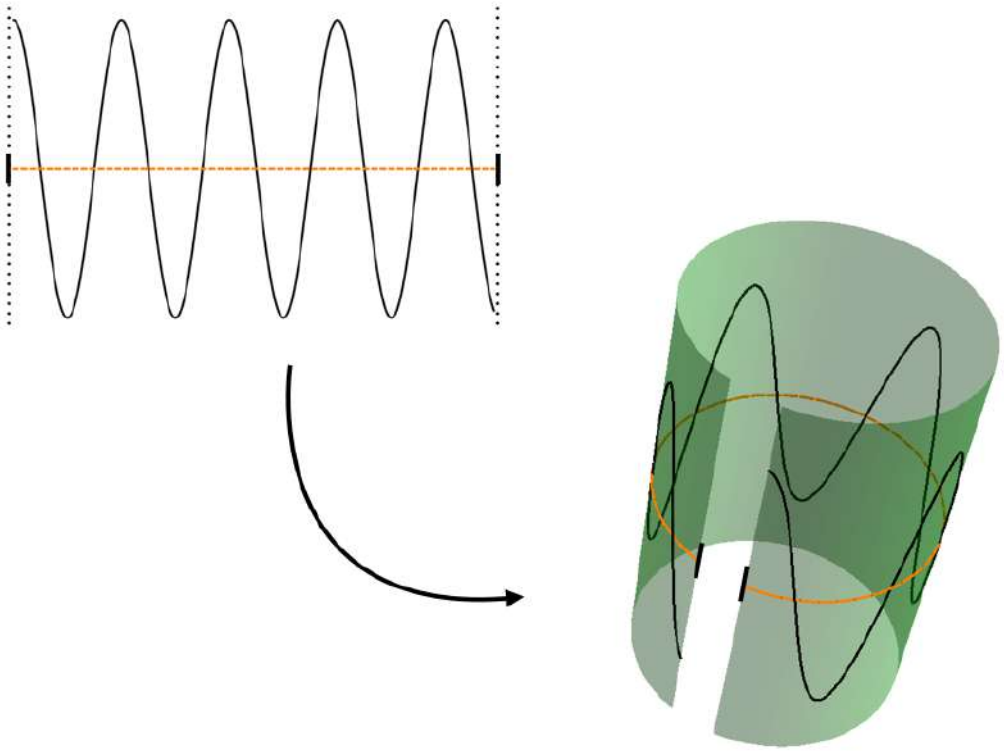

Figure 1.22: After the bending, the functions defined over the interval transform as in figure.

boundary conditions. This phase encodes the properties of the junction like the material it is made of, or its width. In particular, as we are going to discuss in the next chapter, these effects can be used in a Josephson junction and in superconducting quantum interference devices in order to get different quantum boundary conditions [Pol+09; Paa+09].
Eventually, the following non-diagonal unitary matrix describes a delta like potential settled on a point of a circle with intensity g [TFC00; FT01; CFT01]:

$$U_g = \frac{1 - i\,g}{1 + g^2} \begin{pmatrix} ig & 1 \\ 1 & ig \end{pmatrix}. \tag{1.87}$$

The boundary conditions associated to this unitary matrix can be used to describe effectively the quantum dynamics on a circular superconducting quantum device (SQUID) with a Josephson junction. It is exactly the non-

diagonal nature of U_g which takes into account the tunneling effects across the junction.

1.7 Physical interpretation of boundary conditions: a scattering approach

In the previous section we classified all self-adjoint extensions of the Laplacian on an interval and, in particular, we met again with Dirichlet and Neumann conditions. It is legitimate to ask what would be the physical meaning of these conditions. We also analyzed the role of boundary conditions in the light of unitary preservation, and stressed the necessity of deforming the interval topology into the circle one, in order to make the transition"what comes out from one end must return to the other" a physical one (Figure 1.22).

We would like to show, through the use of scattering techniques, what is the physical meaning of the requests made so far, e.g. the vanishing of the wave function or of its derivative at one endpoint. We take the Laplacian defined over its maximal domain on an interval $[0,1]$, that is $H^2[0,1]$, and study what happens in a neighbourhood of 0.

In order to do so, we consider a plane wave $\mathrm{e}^{-i\,k\,x}$, which is in $H^2[0,1]$, coming from the right (region I), which in part gets reflected (region I) and in part transmitted (region II). (Figure 1.23)

Let R be the reflection coefficient and T the transmission one, so that the wavefunction can be written as:

$$\psi(x) = \begin{cases} \psi_I(x) = e^{-i\,k\,x} + Re^{i\,k\,x} & x \in I, \\ \psi_{II}(x) = Te^{-i\,k\,x} & x \in II \end{cases} \tag{1.88}$$

We start analyzing the physical meaning of $\psi(0) = 0$. By imposing this

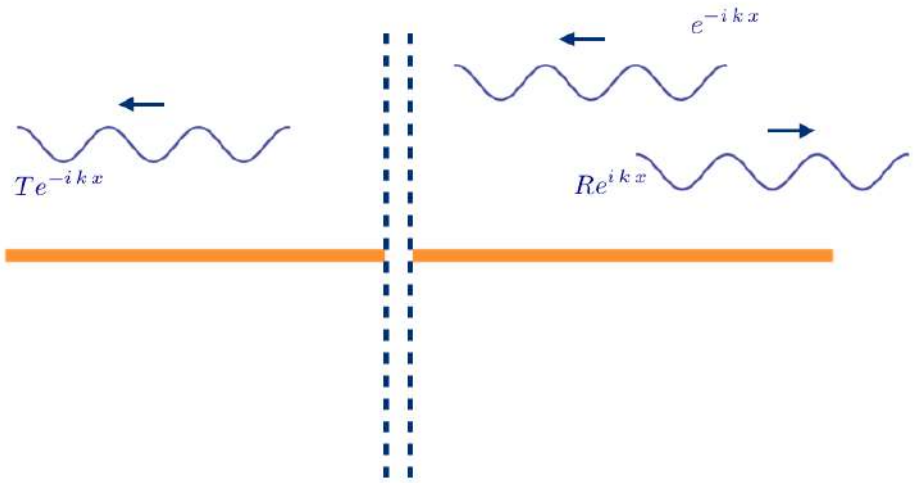

Figure 1.23: Scattering of a plane wave e^{-ikx} against one of the boundary's ends.

condition in (1.88) we find that:

$$\begin{cases} R = -1 \\ T = 0 \end{cases} . \tag{1.89}$$

Physically this means that the plane wave scatters against a hard wall, no transmission takes place, and it is completely reflected. In the reflection process it acquires a π phase like in the classical case of scattering of light against a mirror. In the physical interpretation of $\psi(0) = 0$, we can always think of bending our interval into a ring with a junction that consists of an infinitely high wall.
Next, we move on to $\psi'(0) = 0$ and find that:

$$\begin{cases} R = 1 \\ T = 0 \end{cases} . \tag{1.90}$$

In this case as well, the incoming wave gets completely reflected by a hard wall, but in this case in the reflection process it does not acquire any additional phase.

In Chapter 2 we will prove that there exists a non trivial geometric phase for a free particle described by a Laplacian with the following boundary conditions:

$$\psi(0) = \eta\psi(1), \qquad \overline{\eta}\psi'(0) = \psi'(1). \tag{1.91}$$

We have already remarked that in order to give a physical meaning to our boundary problems we need to bend our segment so that the interval ends are brought close to each other to form the two sides of a junction, so that the conditions we need to impose are:

$$\begin{cases} \psi_I(0) = \eta\,\psi_{II}(0) \\ \overline{\eta}\,\psi_I'(0) = \psi_{II}'(0) \end{cases}, \tag{1.92}$$

which lead to the following coefficients:

$$R = \frac{|\eta|^2 - 1}{1 + |\eta|^2}, \tag{1.93}$$

$$T = \frac{2\,\overline{\eta}}{1 + |\eta|^2}. \tag{1.94}$$

In the periodic case, $\eta = 1$, where we can identify the interval ends, the incident wave is completely transmitted through the junction, that is the particle is freely moving on a circle. In the antiperodic case, instead, that is $\eta = -1$, again the wave is completely transmitted, but by crossing the junction it acquires an additional π phase.
Interestingly the coefficients found above are the same that we already found in the ispection of self-adjoint extensions of the Laplacian on the interval, that is:

$$U = -\begin{pmatrix} R & T^* \\ T & -R \end{pmatrix}. \tag{1.95}$$

It is worth noticing that in the case studied above both R and T were independent of k. However, if we had started from conditions mixing functions and derivatives as:

$$\psi(0) = \eta\,\psi'(1), \tag{1.96}$$

then the reflection and transmission coefficients would explicitly depend on the wave number.

Chapter 2

Moving Walls and Geometric Phases

In this chapter we are going to unveil the existence of a non-trivial Berry phase associated to the dynamics of a quantum particle in a one dimensional box with moving walls [Fac+16]. In order to preserve unitarity a suitable choice of boundary conditions has to be made. For these boundary conditions we are going to explicitly compute the geometric phase associated to the adiabatic evolution of the system. In particular, the unboundedness of the Hamiltonian describing the system leads to a natural prescription of renormalization for divergent contributions arising from the boundary.

2.1 Boundary Conditions and geometric phases

The case of a nonrelativistic quantum particle confined in a one-dimensional box with moving walls subject to Dirichlet boundary conditions has been investigated in great detail in [Di +16].
In this chapter we consider more general boundary conditions and study the geometric phases that emerge. The boundary conditions we focus on are

those consistent with the unitarity of the dynamics as well as with dilation symmetry.

Geometric phases were investigated by Berry and Wilkinson [BW84] who considered the behaviour of the eigenfunctions of the Laplacian in a two dimensional region with a triangular boundary with Dirichlet boundary conditions, when the shape of the region was varied adiabatically. This study revealed the existence of "diabolical points", shapes which have an accidental degeneracy in the spectrum.

Varying the shape of the region in a small circuit around the diabolical point led to a reversal in the sign of the eigenfunction. Similar effects were also noticed earlier in molecular physics [HL63] as explained in the book by Shapere and Wilczek [SW03]. These sign reversals were an early example of a geometric phase. In these problems the geometric phase is essentially of topological origin. In fact, due to the time reversal symmetry of the problem, wave functions can be chosen to be real and this constrains all geometric phases to be 1 or -1. In a later work by Berry, the time reversal symmetry was broken by the introduction of magnetic fields and this led to the discovery of the full geometric phase [Ber84], which has been subsequently studied and generalized in many directions [AA87; SB88] and widely applied [Boh+03; CJ04].

In this chapter, unlike the example studied by Berry and Wilkinson, which is two-dimensional, we are going to consider a free quantum particle in a one-dimensional box subject to general boundary conditions, which (apart from some special cases) violate time reversal symmetry.

The location of the boundaries is adiabatically varied by translations and dilations, which gives us a two parameter space of variations. As a result we are going to find that there is a geometric phase and we are going to compute the two -form on the parameter space.

Interestingly enough, it turns out that this two-form is the area form of a hyperbolic half-plane. This is at variance with the curvature of the original example (a spin in a magnetic field) in Berry's seminal work [Ber84]. The latter was the area two-form of a sphere which is known to be associated to the degeneracy occurring at zero magnetic field. Moreover, the eigenvalue

crossings can be associated to a Berry curvature with a similar geometry. Surprisingly, our model presents no crossing and the nontrivial geometric phase is associated to a hyperbolic geometry.

2.2 The adiabatic theorem and geometric phases

From the axioms of quantum mechanics we know that given a quantum system one can associate to it a self-adjoint operator, the Hamiltonian, which, among other things, determines the time-evolution of the system. In order to investigate how the system evolves in time one needs to solve the Schrödinger equation:

$$i\hbar\partial_t\psi(t) = H(t)\psi(t), \tag{2.1}$$

where $\psi(t)$ is some state, i.e. a unit vector in a Hilbert space, e.g. $L^2(\mathbb{R})$. The solutions of the Schrödinger equation in the time-independent case are well-known in literature [Mes61; Sak93], while in the time-dependent one they need more care.

In the most general situations it is not possible to write down an explicit solution of (2.1), due to the operatorial nature of the Hamiltonian. However, sometimes we are interested in slowly-changing systems so that, in the so-called *adiabatic approximation*, one can give an approximate solution to the Schrödinger equation.

Adiabaticity plays a fundamental role in physics since it is at the borderline between statics and dynamics; indeed, it keeps track of infinitely slow dynamical effects, so that it is no longer static but its evolution is extremely slow. Adiabatic evolution has, of course, its counterpart in classical mechanics [Arn97] where one considers adiabatic invariants, which for time-dependent Hamiltonians are the objects closest to conserved quantities. The construction of such invariants, which approximate well-enough integrals of motion, can be accomplished as a result of the adiabatic approximation.

A first formulation of the adiabatic theorem was given by Born and Fock [BF28], although Kato's seminal paper [Kat50] represents a cornerstone in

the geometrical interpretation of such a slow evolution.
A general formulation of the adiabatic problem is the following. Let $\tau > 0$ be a fixed constant representing the total time of the evolution and let us rescale the time coordinate $t \to s = t/\tau$, so that $s \in [0, 1]$, and the Schrödinger equation reads:

$$i\partial_s \psi_\tau(s) = \tau H(s)\psi_\tau(s). \tag{2.2}$$

We are now interested in what happens in the limit $\tau \to \infty$. There are several forms of the theorem, which all depend on the regularity properties of the given data, but share the same structure. Indeed, given a suitable family $P(s)$ of spectral projections of $H(s)$, we suppose that the initial state $\psi_\tau(0) \in \text{Range}P(0)$, then for some $\gamma \geq 0$:

$$\text{dist}\left(\psi_\tau(s), \text{Range}P(s)\right) \leq o(\tau^\gamma). \tag{2.3}$$

In other words if we start the evolution in an eigenspace, then the dynamically evolved state can be approximated as much as we want by a state in the final evolved eigenspace.
One question may arise naturally: What is the meaning of a "slowly-varying" time evolution? Of course one needs to define a reference time-scale, so that the expression "fast" and "slow" are well-posed. If we start from an isolated eigenvalue in the spectrum, we can define an intrinsic temporal scale, and we can also estimate how good our approximation is. In the gapless case the theorem holds [AE99], as well, but since there is no characteristic time scale we cannot infer about the rate at which our approximation is reached. For some recent applications of adiabaticity in terms of shortcuts for scale invariant driving see [DJC14].

2.2.1 The Born - Fock approximation

In 1928 [BF28] Born and Fock proved a version of the theorem for an Hamiltonian with a non degenerate and discrete spectrum:

$$H(t)\, u_n(t) = E_n(t) u_n(t) \tag{2.4}$$

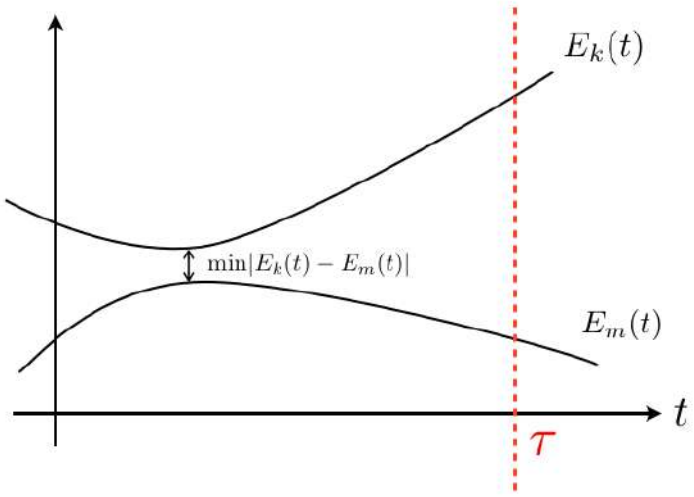

Figure 2.1: Adiabatic evolution is concerned with comparing two temporal scales, an intrinsic one which is related to the distance between close energy levels and an external one, say τ.

with the choice of normalized eigenvectors. They proved that, if $\psi(0) = u_n(0)$, then, the evolved state at later times can be well-approximated with the evolved eigenstate, say $u_n(t)$, modulo an extra phase factor:

$$\psi(t) = \exp(i\,\phi_n(t)) \exp\left(-\frac{i}{\hbar}\int_0^t E_n(s)\mathrm{d}s\right) u_n(t), \tag{2.5}$$

It is fundamental to remark one aspect of adiabatic evolution.
First, time evolution of the systems we are going to study will be implemented by some external parameters, (see for istance section 2.2.2), for example the well known case of a spin one-half particle into a slowly varying magnetic field, whose intensity is kept constant.
In the analysis of adiabatic evolution there are two temporal scales which need to be taken into account. The first one, τ, is the temporal scale associated to the time evolution of the parameters, or, in other words, it tells us how rapidly the Hamiltonian varies with time. In the above example, it corresponds to the period of rotation of the magnetic field. Moreover, there is an intrinsic time scale, which is related to the difference between two close

energy levels (see Figure (2.1)) and it is proportional to the intensity of the magnetic field, or more generally to $\|H\|$, and consequently to the eigenvalues of the Hamiltonian. The idea of adiabatic evolution is the following: we let the magnetic field vary so slowly (τ very large) that no transition between energy levels can occur, or alternatively we increase the difference between the energy levels and let B vary at a given pace. Indeed, what physically really matters is the ratio between the two time scales. Adiabaticity, then, means that the external time-dependent parameters are not that fast to provoke a jump between close energy levels during the evolution.

2.2.2 The Berry phase

For fifty years the contribution of the additional phase ϕ_n in equation (2.5) was ignored by the physics community and believed to be unphysical, since it could have been neglected through a gauge transformation of the basis eigenvectors. Indeed if we perform a gauge transformation

$$u_n(t) \to u'_n(t) = e^{i\,\lambda_n(t)} u_n(t) \qquad \lambda_n : \mathbb{R} \to \mathbb{R}, \tag{2.6}$$

then, equation (2.4) will hold for the transformed states as well. Using the gauge freedom, we could have chosen the states:

$$\tilde{u}_n(t) = e^{i\phi_n(t)} u_n(t), \tag{2.7}$$

and the state in (2.5) can be rewritten as:

$$\psi(t) = \exp\left(-\frac{i}{\hbar}\int_0^t E_m(s)\mathrm{d}s\right)\tilde{u}_n(t), \tag{2.8}$$

so that no extra contribution seems to appear. As we are going to revise, there are some cases when the latter machinery fails and it turned out that an extra purely geometrical phase is indeed needed. This extra contribution is linked to the geometrical properties of the quantum evolution.

Indeed, we start with a curve $\mathcal{C}$ in the parameter space $\mathcal{M}$:

$$t \to x_t \in \mathcal{M} \tag{2.9}$$

and consider a family of parameter dependent Hamiltonians defined over the parameter space. We suppose that $H(x)$ admits a purely discrete spectrum over the whole $\mathcal{M}$:

$$H(x)u_n(x) = E_n(x)u_n(x) \ , \qquad \langle u_n(x), u_m(x)\rangle = \delta_{n,m} \quad \forall x \in \mathcal{M}. \tag{2.10}$$

Notice that the eigenvectors in (2.10) are not uniquely determined since one could perform the gauge transformation:

$$u_n(x) \to \tilde{u}_n(x) = e^{i\alpha_n(x)}u_n(x), \tag{2.11}$$

$$\alpha_n : \mathcal{M} \to \mathbb{R}, \tag{2.12}$$

leaving equation (2.10) unaltered.
We, now, focus our attention on the n-th eigenspace, assume it is not degenerate and apply the adiabatic approximation. We consider the rank-one projection $P_n(x)$ and build up a fiber in x:

$$\mathcal{H}_n(x) = \mathrm{Ran}\, P_n(x) = \{\alpha\, u_n(x) : \alpha \in \mathbb{C}\}. \tag{2.13}$$

Next we investigate the dynamical evolution and consider the restriction of the family of Hamiltonians in (2.10) to the chosen path, so that time-dependence will be implemented by the following composition:

$$t \to x_t \in \mathcal{M} \to H(x_t). \tag{2.14}$$

Suppose we start with a vector $\psi(0) = u_n(x_0)$ and let it evolve adiabatically, so that for every t we can approximate the true evolved state with a state in the n-th eigenspace:

$$\psi(t) \in \mathcal{H}_n(x_t). \tag{2.15}$$

If we consider a cyclic evolution of parameters, that is to say $\mathcal{C}$ a closed path

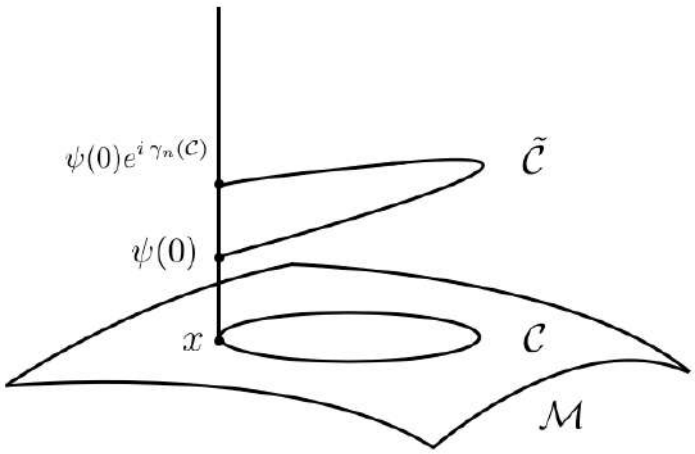

Figure 2.2: Although the physical system is subdued to a cyclical evolution of the parameter x in $\mathcal{M}$, the wavefunction ψ, crossing the horizontal lift $\tilde{\mathcal{C}}$ of $\mathcal{C}$, can be different from the initial one, say $\psi(0)$ when the external parameter returns to its original value. In this case the wavefunction has acquired an extra phase factor.

on $\mathcal{M}$, then after a turn around the state $\psi(T)$ still belongs to $\mathcal{H}_n(x_0)$ but it may differ from $\psi(0)$ by a phase factor:

$$\psi(T) = e^{i\gamma}\psi(0). \tag{2.16}$$

Naively one could think that this phase γ is solely determined by the dynamical evolution of the system, that is:

$$\gamma \propto \int_0^T E_n(t)\mathrm{d}t, \tag{2.17}$$

but, as Berry discovered in 1984 [Ber84], although earlier anticipations can be found in Pancharatnam [Pan56], there exists an extra purely geometrical contribution depending only on the properties of the manifold and on the chosen path. From the adiabatic approximation (equation (2.5)) we can write:

$$\psi(t) = \exp\left(-\frac{i}{\hbar}\int_0^T E_n(\tau)\,\mathrm{d}\tau\right) e^{i\phi_n(t)}\,u_n(x_t)\,, \tag{2.18}$$

where:

$$\dot{\phi_n} = i \langle u_n, \mathrm{d}u_n \rangle. \tag{2.19}$$

We now define the following one-form:

$$\mathcal{A}^{(n)} := i \langle u_n, \mathrm{d}u_n \rangle. \tag{2.20}$$

Once defined the 1-form above, we can solve equation (2.19) integrating it over the path $\mathcal{C}$, so that the geometrical contribution, known as the *Berry phase* is given by:

$$\gamma_n(\mathcal{C}) := \phi_n(T) = \oint_{\mathcal{C}} \mathcal{A}^{(n)}. \tag{2.21}$$

The total phase shift γ can be explicitly split into a dynamical and a geometrical part :

$$\gamma = -\frac{1}{\hbar} \int_0^T E_n(\tau) \mathrm{d}\tau + \gamma_n(\mathcal{C}). \tag{2.22}$$

We remark that $\hbar$ would appear in the dynamical phase, but not in the geometrical phase. This is a sign of the fact that $\gamma_n(\mathcal{C})$ is independent of the chosen evolution, but it is rather an intrinsic geometrical property, as proved by [AA87; SB88]. From the Stokes theorem (Figure 2.3) we can transform the circulation of $\mathcal{A}^{(n)}$ into a flux integral:

$$\gamma_n(\mathcal{C}) = \int_\Sigma \mathcal{F}^{(n)}, \tag{2.23}$$

where Σ is a surface whose boundary $\partial\Sigma$ is exactly the closed curve $\mathcal{C}$ and $\mathcal{F}^{(n)}$ is given by the exterior differential of $\mathcal{A}^{(n)}$:

$$\mathcal{F}^{(n)} = \mathrm{d}\mathcal{A}^{(n)}. \tag{2.24}$$

Under a gauge transformation (2.11) the one-form $\mathcal{A}^{(n)}$ transforms like a gauge potential of electrodynamics:

$$\mathcal{A}^{(n)} \to \mathcal{A}'^{(n)} = \mathcal{A}^{(n)} - \mathrm{d}\alpha_n, \tag{2.25}$$

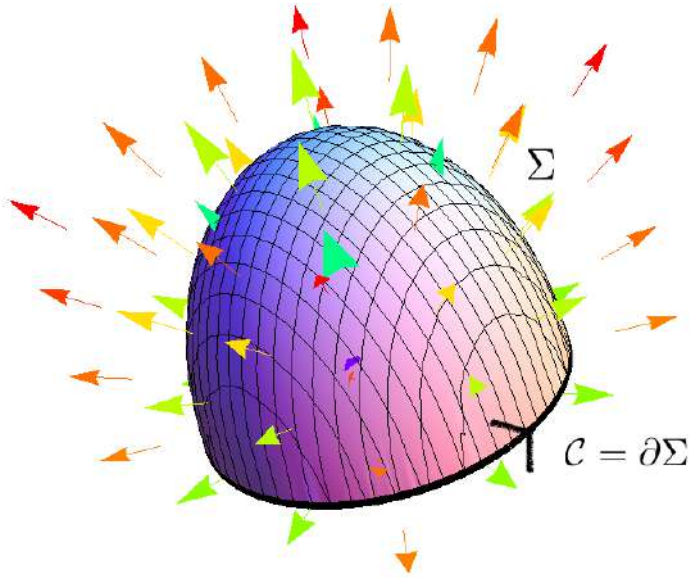

Figure 2.3: Stokes theorem: the flux through Σ equals the circulation on $\partial\Sigma$.

while:

$$\mathcal{F}'^{(n)} = \mathcal{F}^{(n)}, \tag{2.26}$$

due to the identity $\mathrm{d}^2\alpha_n = 0$.
Equation (2.26) shows that $\mathcal{F}^{(n)}$ is a gauge-invariant quantity, as well as the Berry phase $\gamma_n(\mathcal{C})$ due to equation (2.23).
Again, in analogy with classical electrodynamics the 2-form $\mathcal{F}^{(n)}$ plays the role of the magnetic field, whose flux (in our case the Berry phase), is invariant under gauge transformations. This analogy is extremely fruitful since the above derivation can be understood in terms of connections over a principle fiber bundle, which is a powerful tool in gauge theories [Sim83].

2.3 The framework

As already remarked the set of all the possible physical realizations of a free quantum particle in a one-dimensional box, say $I = [a, b]$, $a, b \in \mathbb{R}$, $b > a$, is

in a one-to- one correspondence with the set of 2×2 unitary matrices:

$$\begin{aligned} &H_U\psi = -\frac{\hbar^2}{2m}\psi'', \\ &\mathrm{D}(H_U) = \{\psi \in H^2(I) :\ \mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}\}. \end{aligned} \tag{2.27}$$

where U is a unitary 2×2 matrix and:

$$\varphi = \begin{pmatrix} \psi(a) \\ \psi(b) \end{pmatrix}, \qquad \dot{\varphi} = \begin{pmatrix} -\psi'(a) \\ \psi'(b) \end{pmatrix}. \tag{2.28}$$

w we would like to extract and parametrize a particular subset of boundary conditions which are invariant under dilations and will be useful in the following. The set we are looking for is made up by all those boundary conditions which do not mix functions with derivatives at the boundary, that is of the form

$$\begin{cases} \alpha\,\psi(a) + \beta\,\psi(b) = 0, \\ \gamma\,\psi'(a) + \delta\,\psi'(b) = 0, \end{cases} \tag{2.29}$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{C}$. It is easy to show that the conditions that have to be satisfied by the former four parameters in order to represent a self-adjoint extension of the Hamiltonian on the interval $I = [a, b]$ are

$$\beta\bar{\delta} = \alpha\bar{\gamma}. \tag{2.30}$$

If we set $\eta = -\beta/\alpha$, the desired boundary conditions read

$$\begin{cases} \psi(a) = \eta\,\psi(b), \\ \overline{\eta}\psi'(a) = \psi'(b), \end{cases} \tag{2.31}$$

and the unitary matrix in (2.27) associated to this self-adjoint extension is provided by

$$U = \begin{pmatrix} \frac{1-|\eta|^2}{1+|\eta|^2} & \frac{-2\eta}{1+|\eta|^2} \\ \frac{-2\overline{\eta}}{1+|\eta|^2} & \frac{|\eta|^2-1}{1+|\eta|^2} \end{pmatrix}. \tag{2.32}$$

Some comments are in order. If $\eta = \pm 1$ we obtain periodic and antiperiodic

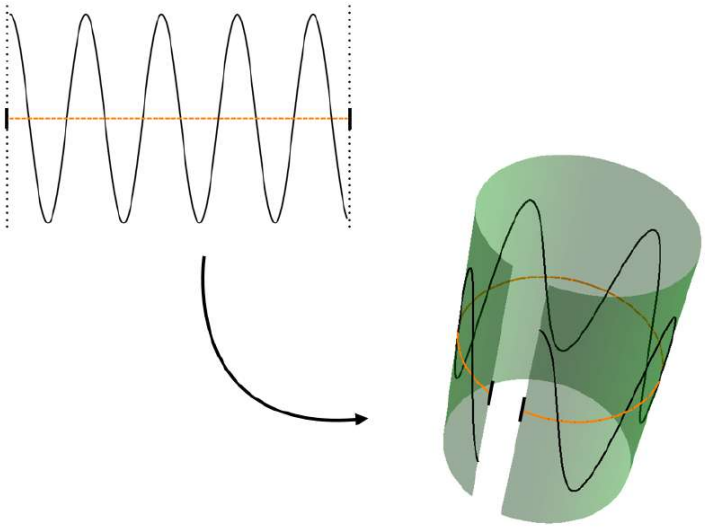

Figure 2.4: After the bending, the functions defined over the interval transform as in figure.

boundary conditions, while for $\eta = 0$ or $\eta = \infty$ mixed Dirichlet and Neumann conditions arise. However, pure Dirichlet or Neumann conditions cannot be reached by our parametrization. Thus, the family in (2.32), which we denote by $\{\mathcal{U}(\eta)\}_{\eta\in\mathbb{C}_\infty}$, where $\mathbb{C}_\infty = \mathbb{C} \cup \{\infty\}$, does not exhaust the whole set of dilation-invariant boundary conditions, which is instead provided by

$$\{\mathcal{U}(\eta)_{\eta\in\mathbb{C}_\infty}, \mathbb{I}, -\mathbb{I}\}. \tag{2.33}$$

Moreover, it is worth noticing that the set $\{\mathcal{U}(\eta)\}$ does not form a subgroup of U(2). In fact, the family in (2.32) does not support a group structure because it has topology S^2 which is not parallelizable.
From a physical perspective the boundary conditions in (2.31) are nonlocal, since they connect the value of the wave function at one end of the interval with its value at the other end.
As discussed in the previous chapter, a physical realization of them requires that the interval be bent into a ring with the two ends forming a tunneling junction through which the wave function can acquire a phase given by (2.32). See Fig. 2.4.

This can be experimentally implemented by means e.g. of superconducting quantum interference devices, where the properties of the Josephson junction are suitably chosen to give the required phase [Aso+13].
Another possible experimental realisation is offered by recent developments in cold atom physics. It is possible to trap Bose Einstein condensates in optical traps and manipulate them by altering the shape and size of the trap. By detuning the laser frequency one can introduce optical barriers to bisect a circular optical trap. A BEC in such a trap would give us the same tunnelling properties as a Josephson junction [Cat+01] permitting us to simulate various boundary conditions.

2.4 Moving and fixed walls

We start by generalizing the problem of a particle of mass m in a one dimensional box with moving walls subject to Dirichlet boundary conditions (extensively discussed in [Di +16; DF15]) to a larger class of boundary conditions, which we picked out in (2.33). For convenience we parametrize the one dimensional box by

$$I_{l,c} = [c - l/2, c + l/2], \tag{2.34}$$

so that $c \in \mathbb{R}$ is the center of the interval, and $l > 0$ is its length, and consider the Hamiltonian (kinetic energy)

$$\begin{aligned} &H\psi = -\tfrac{\hbar^2}{2m}\psi'', \qquad \psi \in \mathrm{D}_{l,c}, \\ &\mathrm{D}_{l,c} = \left\{ \psi \in H^2(I_{l,c}) : \ \psi\left(c - \tfrac{l}{2}\right) = \eta\psi\left(c + \tfrac{l}{2}\right), \ \bar{\eta}\psi'\left(c - \tfrac{l}{2}\right) = \psi'\left(c + \tfrac{l}{2}\right) \right\}, \end{aligned}$$

where η is a fixed complex number representing particular boundary conditions (2.31), and $H^2(I_{l,c})$ is the Sobolev space of square integrable functions on $I_{l,c}$, whose first and second derivatives are square integrable functions.
Some comments are necessary. In the previous section we proved that the above boundary conditions yield a good self-adjoint extension of the Hamiltonian on an interval. As already remarked these do not mix the values of

the functions at the border with their derivatives. In what follows we will see that these are the only ones which are invariant under dilations [ILP15a], a crucial property for what we are going to investigate.
Next we take into account the dynamics of this problem by taking smooth paths in the parameter space $(l, c) \in \mathbb{R}_+ \times \mathbb{R}$: $t \mapsto c(t)$ and $t \mapsto l(t)$. Clearly we are translating the box by $c(t)$ and contracting/dilating it by $l(t)$. As underlined in [Di +16] determining the quantum dynamics of this system is not an easy problem to tackle with, since we have Hilbert spaces, $L^2(I_{l(t),c(t)})$, varying with time and we need to compare vectors in different spaces. The standard approach is to embed the time-dependent spaces into a larger one, namely $L^2(\mathbb{R})$, extend the two-parameter family of Hamiltonians (2.35) to this space and try to unitarily map the problem we started with into another one, with a family of time-dependent Hamiltonians on a fixed common domain.
With this end in view we embed $L^2(I_{l,c})$ into $L^2(\mathbb{R})$ in the following way

$$L^2(\mathbb{R}) = L^2(I_{l,c}) \oplus L^2(I_{l,c}^{\mathrm{c}}), \tag{2.35}$$

where $I^{\mathrm{c}} = \mathbb{R} \setminus I$ is the complement of the set I, so that we can consider the extension of the Hamiltonians defined in (2.35) as

$$H(l, c) = \frac{p^2}{2m} \oplus_{l,c} \mathbf{0}, \tag{2.36}$$

where the embedding and the direct sum obviously depend on l and c.

2.4.1 The reduction procedure

Following [Di +16] we recall how to reduce this moving walls problem into a fixed domain one. The composition of a translation $x \to x - c$ and of a subsequent dilation $x \to x/l$ maps the interval $I_{l,c}$ onto

$$I = I_{1,0} = \left[-\frac{1}{2}, \frac{1}{2} \right], \tag{2.37}$$

which does not depend on c and l. Next we need to define a unitary action of both groups on $L^2(\mathbb{R})$. A possible choice is

$$(V(c)\psi)(x) = \psi(x-c), \qquad (W(s)\psi)(x) = \mathrm{e}^{-s/2}\psi(\mathrm{e}^{-s}x), \quad \forall \psi \in L^2(\mathbb{R}), \tag{2.38}$$

and both $c \in \mathbb{R} \to V(c)$ and $s = \ln l \in \mathbb{R} \to W(s)$ form one-parameter (strongly continuous) unitary groups. The factor $\exp(-s/2)$ is consistent with the physical expectation that ψ transforms as the square root of a density under dilation.

In order to make the expression $\ln l$ meaningful, from now on we are going to identify l with a pure number given by the ratio of the actual length of the box and a unit length. The infinitesimal generator of the group of translations is the momentum operator

$$p : D(p) = H^1(\mathbb{R}) \to L^2(\mathbb{R}), \qquad p\psi = -i\hbar\,\psi', \tag{2.39}$$

so that spatial translations are implemented by the unitary group

$$V(c) = \exp\left(-i\,\frac{c}{\hbar}\,p\right), \qquad \forall\, c \in \mathbb{R}. \tag{2.40}$$

Similarly, the generator of the dilation unitary group is given by the virial operator over its maximal domain:

$$x \circ p := \overline{xp - \frac{\mathrm{i}}{2}} = \overline{\frac{1}{2}(xp+px)}, \qquad \mathrm{D}(x\circ p) = \{\psi \in L^2(\mathbb{R}) \,|\, x\psi' \in L^2(\mathbb{R})\}, \tag{2.41}$$

where $\overline{A}$ denotes the closure of the operator A. Dilations on $L^2(\mathbb{R})$ are, thus, implemented by

$$W(s) = \exp\left(-\mathrm{i}\,\frac{s}{\hbar}\,x\circ p\right), \qquad \forall\, s \in \mathbb{R}. \tag{2.42}$$

Next, we define the two-parameter family of unitary operators on $L^2(\mathbb{R})$,

which are going to fix our time-dependent problem

$$U(l,c) : L^2(\mathbb{R}) \to L^2(\mathbb{R}), \qquad U(l,c) = W^\dagger(\ln l)V^\dagger(c). \tag{2.43}$$

By this unitary isomorphism we are mapping $H(l,c)$ into

$$H(l) = U(l,c)H(l,c)U^\dagger(l,c) = \frac{p^2}{2ml^2} \oplus \mathbf{0}, \tag{2.44}$$

where we have used the identity

$$W^\dagger(\ln l)\, p\, W(\ln l) = \frac{p}{l}. \tag{2.45}$$

The operators in (2.44) act on the time-independent domain

$$\mathrm{D}(H(l)) = \mathrm{D} \oplus L^2(I^c), \tag{2.46}$$

where $\mathrm{D} = U(l,c)\mathrm{D}_{l,c}$ is given by

$$\mathrm{D} = \left\{ \psi \in \mathrm{H}^2(I) \,:\, \psi\left(-\frac{1}{2}\right) = \eta\psi\left(\frac{1}{2}\right),\ \bar{\eta}\psi'\left(-\frac{1}{2}\right) = \psi'\left(\frac{1}{2}\right) \right\}. \tag{2.47}$$

We have thus achieved our goal, that is mapping the initial family of Hamiltonians with time-dependent domains into a family with a common fixed domain of self-adjointness.
This has been possible thanks to the unitary operator (2.43) and, most importantly, to the choice of dilation-invariant boundary conditions (2.35) as discussed in the previous section. We have taken into account those boundary conditions (2.31) which do not mix derivatives and functions at the boundary: these are the only ones which leave the transformed domain $\mathrm{D} = U(l,c)\mathrm{D}_{l,c}$ in (4.10) time-independent.

2.5 The Berry phase factor

The main objective of this section will be to exhibit a non-trivial geometric phase associated to a cyclic adiabatic evolution of the physical system

described in section 2.4.

Let $\mathcal{C}$ be a closed path in the parameter space $(l, c) \in \mathbb{R}_+ \times \mathbb{R}$. Let the n-th energy level be non degenerate; then, in the adiabatic approximation, the Berry phase associated to the cyclical adiabatic evolution is given by

$$\Phi_n = \oint_{\mathcal{C}} \mathcal{A}^{(n)} = \mathrm{i} \oint_{\mathcal{C}} \langle \psi_n | \mathrm{d}\psi_n \rangle, \tag{2.48}$$

where ψ_n is the eigenfunction associated to the n-th eigenvalue, d is the external differential defined over the parameter manifold $\mathbb{R}_+ \times \mathbb{R}$, and

$$\langle \psi_n | \mathrm{d}\psi_n \rangle = \int_{\mathbb{R}} \overline{\psi_n(x)} (\mathrm{d}\psi_n)(x) \mathrm{d}x. \tag{2.49}$$

In our case $\mathrm{d}\psi_n$ reads

$$(\mathrm{d}\psi_n)(x) = \left(\frac{\partial}{\partial l} \psi_n \right)(x) \mathrm{d}l + \left(\frac{\partial}{\partial c} \psi_n \right)(x) \mathrm{d}c. \tag{2.50}$$

A technical difficulty arises from equations (2.48)-(2.50). In this section we are going to show that, for fixed η, the eigenfunctions $\{\psi_n\}_{n \in \mathbb{N}}$ determine an orthonormal basis in $L^2(\mathbb{R})$. However, in general the derivatives in (2.50) do not belong to $L^2(\mathbb{R})$ so that the integral in (2.49) is ill-posed and needs a prescription of calculation. No doubt, the ill-posedness of (2.48) is due to the presence of a boundary in our system.

First we need to determine the spectral decomposition of the Hamiltonian we started with in (2.35) or equivalently in (2.36). Of course this would be a difficult problem to handle, but thanks to the unitary operator in (2.43) we can move on to the Hamiltonians with fixed domain, compute the spectral decomposition and then make our way unitarily back to the problem with time-dependent domain. Therefore, we need to solve the eigenvalue problem

$$-\frac{\hbar^2}{2ml^2} \phi''(x) = \lambda \phi(x), \tag{2.51}$$

where $\phi \in \mathrm{D}$ in (4.10) and $\lambda \in \mathbb{R}$. The spectral decomposition will heavily rely on the choice of the parameter η, which, as already stressed, represents

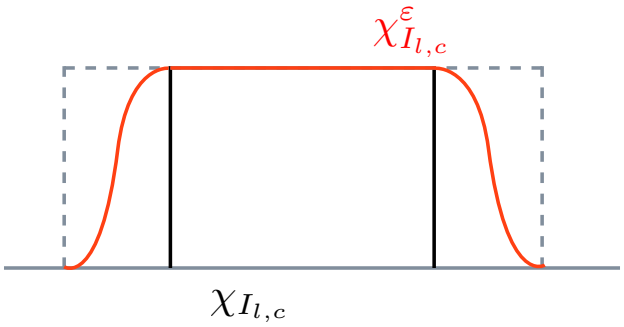

Figure 2.5: Regularized characteristic function (2.55).

a particular choice of boundary condition. If $\eta \neq \pm 1$ the spectrum is non-degenerate, and the normalized eigenfunctions have the form

$$\phi_n(x) = \sin(k_n x) + \mathrm{e}^{i\,\alpha} \cos(k_n x), \qquad n \in \mathbb{Z}, \tag{2.52}$$

where

$$\alpha = \mathrm{Arg}\left(\frac{1+\eta}{1-\eta}\right), \qquad k_n = 2n\pi + 2\arctan\left|\frac{1-\eta}{1+\eta}\right|, \qquad n \in \mathbb{Z}, \tag{2.53}$$

so that the dispersion relation ($\lambda = k^2\hbar^2/2ml^2$) reads

$$\lambda_n = \frac{2\hbar^2}{ml^2}\left(n\pi + \arctan\left|\frac{1-\eta}{1+\eta}\right|\right)^2, \qquad n \in \mathbb{Z}. \tag{2.54}$$

2.5.1 A first regularization prescription

In this subsection we briefly explain the need for a regularization prescription for the eigenfunctions of our Hamiltonian, in order for the derivatives in (2.50) to be well defined.

Let φ be an arbitrary function belonging to $L^2(I^{\mathrm{c}})$, where $I^{\mathrm{c}} = \mathbb{R} \setminus I$ is the complement of the set I; φ is clearly an eigenfunction of the $\mathbf{0}$ operator on $L^2(I^{\mathrm{c}})$ with zero eigenvalue. Therefore we can extend ϕ_n to an eigenfunction of (2.36), $\psi_n = \phi_n \oplus \varphi$, which can be conveniently chosen to be a test function: $\psi_n \in \mathcal{D}(\mathbb{R})$, the space of smooth functions with compact support. To make it explicit, let us exhibit a construction of $\psi_n(x; l, c)$.

Let $\tilde{\phi}_n(x;l,c)$ be a smooth extension of $\phi_n(x;l,c) \in \mathrm{D}_{l,c} \subset L^2(I_{l,c})$ to the whole real line. Roughly speaking our eigenfunction can be written as the restriction of this extension, namely $\tilde{\phi}_n(x;l,c)\chi_{I_{l,c}}(x)$, where $\chi_A(x)$ is the characteristic function of the set A [$\chi_A(x) = 1$ if $x \in A$, and $= 0$ otherwise], showing why divergent contributions arise from the boundary when taking derivatives. So the idea which underlies the following discussion is to regularize the contribution of the characteristic function $\chi_{I_{l,c}}$.
Let $\rho(x)$ be a nonnegative monotone decreasing function which belongs to $C^\infty([0,\infty))$, moreover we require that $\rho(0) = 1$, $\rho(1) = 0$ and all the derivatives of higher order satisfy $\rho^{(n)}(0) = 0$ for $n \geq 1$. We are going to paste two contracted copies of the latter to $\chi_{I_{l,c}}$, such that the final result would be as in Figure 2.5. Given $\varepsilon > 0$ we define the regularized characteristic function of $I_{l,c}$ as follows:

$$\chi^{\varepsilon}_{I_{l,c}}(x) = \begin{cases} 1, & \text{for } x \in I_{l,c} \\ \rho\left(\frac{|x-c|-l/2}{\varepsilon}\right) & \text{for } x \notin I_{l,c}, \end{cases} \tag{2.55}$$

which is a test function, $\chi^{\varepsilon}_{I_{l,c}} \in \mathcal{D}(\mathbb{R})$. In light of the previous discussion we choose the following functions and show that they are eigenfunctions for the Hamiltonian (2.36):

$$\psi_n(x;l,c) = \tilde{\phi}_n(x;l,c)\ \xi_\varepsilon(x;l,c), \qquad \varepsilon > 0, \tag{2.56}$$

where

$$\xi_\varepsilon(x;l,c) = \frac{1}{\|\tilde{\phi}_n\ \chi^{\varepsilon}_{I_{l,c}}\|}\chi^{\varepsilon}_{I_{l,c}}(x). \tag{2.57}$$

See Figure 2.6.
Even if $\tilde{\phi}_n \notin L^2(\mathbb{R})$, this will not alter the desired regularity property and the integrability condition of (2.56). Clearly (2.56) is still an eigenfunction of (2.36) because $\psi_n|_{I_{l,c}} = \phi_n$ is an eigenfunction of the Hamiltonian defined in (2.35) and $\psi_n|_{I^c_{l,c}}$ is trivially an eigenfunction of the $\mathbf{0}$ operator with null eigenvalue. Moreover, from the explicit expression in (2.57) this eigenfunction is normalized.

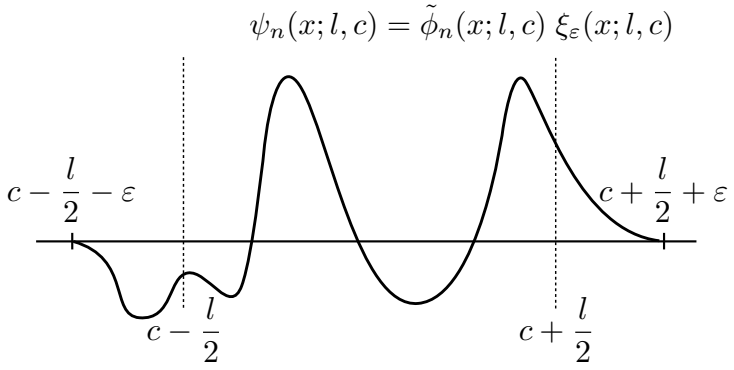

Figure 2.6: The regularization procedure (2.56).

In this renormalization scheme, which is needed for the definiteness of (2.50), we are first embedding $\mathrm{D}_{l,c} \subset L^2(I_{l,c})$ into $L^2(\mathbb{R})$ and then regularizing the boundary contribution through the introduction of the regularizer ρ.
Now it is essential to observe that

$$\lim_{\varepsilon\to 0} \tilde{\phi}_n(x;l,c)\,\xi_\varepsilon(x;l,c) = \tilde{\phi}_n(x;l,c)\,\chi_{I_{l,c}}(x) = \phi_n(x;l,c) \oplus 0, \tag{2.58}$$

that is the eigenfunction of a particle confined in $I_{l,c}$. Here, the convergence of the limit is pointwise and, by dominated convergence, in $L^2(\mathbb{R})$.

2.5.2 The abelian phase: the non degenerate case

We are now in the right position to compute (2.49) for $\varepsilon > 0$, which is well posed, and then take the limit $\varepsilon \to 0$. We start by considering separately both the terms in

$$\langle \psi_n | \mathrm{d}\psi_n \rangle = \left(\int_{\mathbb{R}} \overline{\psi_n(x)} \frac{\partial}{\partial l} \psi_n(x) \mathrm{d}x \right) \mathrm{d}l + \left(\int_{\mathbb{R}} \overline{\psi_n(x)} \frac{\partial}{\partial c} \psi_n(x) \mathrm{d}x \right) \mathrm{d}c, \tag{2.59}$$

which, after an integration by parts, become

$$\int_{\mathbb{R}} \overline{\psi}_n \frac{\partial}{\partial l} \psi_n \mathrm{d}x = \frac{1}{2} \int_{\mathbb{R}} \frac{\partial}{\partial l} |\psi_n|^2 \mathrm{d}x + i\,\mathrm{Im} \int_{\mathbb{R}} \left(\overline{\phi}_n \frac{\partial}{\partial l} \phi_n \right) \xi_\varepsilon^2 \mathrm{d}x, \tag{2.60}$$

$$\int_{\mathbb{R}} \overline{\psi}_n \frac{\partial}{\partial c} \psi_n \mathrm{d}x = \frac{1}{2} \int_{\mathbb{R}} \frac{\partial}{\partial c} |\psi_n|^2 \mathrm{d}x + i\,\mathrm{Im} \int_{\mathbb{R}} \left(\overline{\phi}_n \frac{\partial}{\partial c} \phi_n \right) \xi_\varepsilon^2 \mathrm{d}x. \tag{2.61}$$

By plugging the explicit expressions of the eigenfunctions we find, by dominated convergence, that for $\varepsilon \to 0$

$$\begin{aligned} \mathrm{Im}\int_{\mathbb{R}}\left(\overline{\phi}_n\frac{\partial}{\partial l}\phi_n\right)\xi_\varepsilon^2\mathrm{d}x &= \frac{k_n}{l^3}\sin\alpha\int_{\mathbb{R}}(x-c)\xi_\varepsilon^2(x)\mathrm{d}x \\ &\to \frac{k_n}{l^3}\sin\alpha\int_{I_{l,c}}(x-c)\mathrm{d}x = 0, \qquad (2.62) \\ \mathrm{Im}\int_{\mathbb{R}}\left(\overline{\phi}_n\frac{\partial}{\partial c}\phi_n\right)\xi_\varepsilon^2\mathrm{d}x &= \frac{k_n}{l^2}\sin\alpha\int_{\mathbb{R}}\xi_\varepsilon^2(x)\mathrm{d}x \\ &\to \frac{k_n}{l^2}\sin\alpha\int_{\mathbb{R}}\chi_{I_{l,c}}(x)\mathrm{d}x = \frac{k_n}{l}\sin\alpha. \qquad (2.63) \end{aligned}$$

Moreover, since ψ_n has inherited from $U^\dagger(l,c)$ the right regularity properties, for any $\varepsilon > 0$, one gets

$$\int_{\mathbb{R}}\frac{\partial}{\partial l}|\psi_n|^2\mathrm{d}x = \frac{\partial}{\partial l}\int_{\mathbb{R}}|\psi_n|^2\mathrm{d}x = 0, \qquad \int_{\mathbb{R}}\frac{\partial}{\partial c}|\psi_n|^2\mathrm{d}x = \frac{\partial}{\partial c}\int_{\mathbb{R}}|\psi_n|^2\mathrm{d}x = 0. \tag{2.64}$$

Summing up, we finally get the expression of the Berry one-form:

$$\langle\psi_n|\mathrm{d}\psi_n\rangle = \mathrm{i}\left(\frac{k_n}{l}\sin\alpha\right)\mathrm{d}c, \tag{2.65}$$

which is manifestly not closed yielding a nontrivial Abelian phase. Notice that the one-form derived in (2.65) is purely imaginary, consistently with the general theory of Berry phases [Boh+03]. Moreover it *does* depend on the energy level through k_n in (2.53) and on the boundary conditions through $\sin\alpha$.

As a simple example, we choose a rectangular path $\mathcal{C}$ in the (l,c) half-plane, as shown in Figure 2.7, and compute

$$\Phi_n = \oint_{\mathcal{C}}\mathcal{A}^{(n)} = i\oint_{\mathcal{C}}\langle\psi_n|\mathrm{d}\psi_n\rangle, \tag{2.66}$$

whose only non-trivial contributions are given by the vertical components of

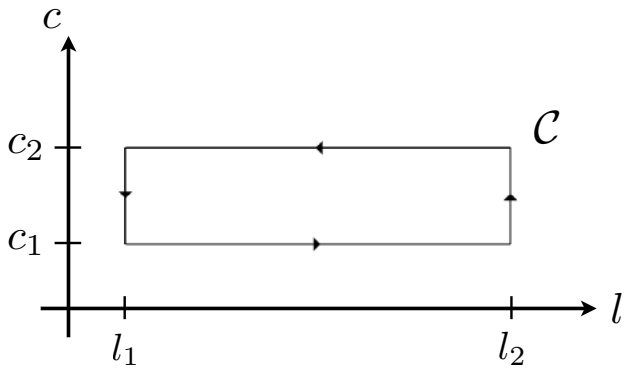

Figure 2.7: The adiabatic path $\mathcal{C}$.

the circuit. The final result is

$$\Phi_n = \oint_{\mathcal{C}} \mathcal{A}^{(n)} = k_n \left(\frac{1}{l_1} - \frac{1}{l_2} \right) (c_2 - c_1) \sin \alpha, \tag{2.67}$$

which, as expected, depends on the particular path chosen. In the spirit of the physical implementation of our system in terms of a ring with a junction (see section 2.3), our cyclic adiabatic evolution could be illustrated as in Figure 2.8.

We have considered the problem of a particle in a box with moving walls with a class of boundary conditions. Unlike the example studied by Berry and Wilkinson (two dimensional region with Dirichlet boundary conditions), our box is one dimensional and we impose more general boundary conditions. We consider situations in which the location and the size of the box are slowly varied. Our problem is complicated by the fact that different points in the parameter space correspond to different Hilbert spaces.

In order to deal with this we need to invoke a larger Hilbert space and exercise care while varying our two parameters. Within this two parameter space we conclude that there is a non-trivial geometric phase. Our boundary conditions in general violate time reversal symmetry, i.e, the complex conjugate of a wave function which satisfies the boundary condition described by η may not satisfy the same boundary condition. In fact, the only boundary conditions that respect time reversal are those where η is real. In this case, we would expect the geometric phase to reduce to the topological phase (which

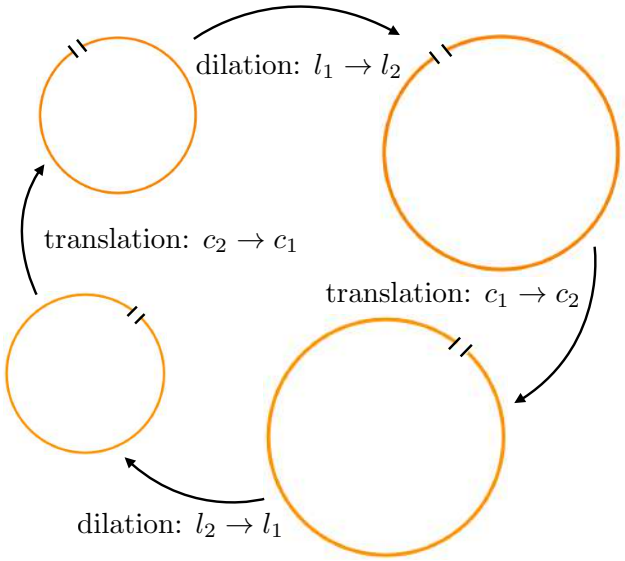

Figure 2.8: Cyclic evolution according to the path drawn in Figure 2.7.

only takes values ± 1). Indeed, when η is real (but not equal to ± 1, which is a degenerate case), α in (2.53) is zero or π.

2.5.3 The Berry curvature

Another interesting aspect provided by this problem is linked to a nontrivial Berry curvature:

$$\mathcal{F}^{(n)} = \mathrm{d}\mathcal{A}^{(n)} = \frac{k_n}{l^2} \sin\alpha \, \mathrm{d}l \wedge \mathrm{d}c. \tag{2.68}$$

The functional form of this phase two-form is suggestive of the area two-form in hyperbolic geometry. The above formula brings to mind, in fact, the curvature of a hyperbolic Riemannian manifold. Indeed, consider the *Poincaré half-plane*, which by definition is the upper-half plane together with the Poincaré metric:

$$\mathrm{d}s^2 = \frac{\mathrm{d}x^2 + \mathrm{d}y^2}{y^2}. \tag{2.69}$$

The half-plane is a model of hyperbolic geometry and if we consider the area form on it we have

$$A = \frac{\mathrm{d}x \wedge \mathrm{d}y}{y^2}, \tag{2.70}$$

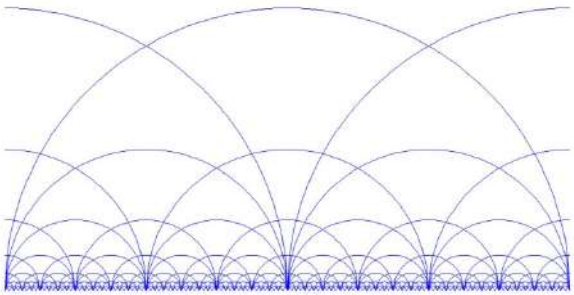

Figure 2.9: Geodesics in the Poncaré half-plane

which has the same structure as the Berry curvature (2.68) of our quantum mechanical model.
As already stated the boundary conditions chosen do not preserve time reversal symmetry as long as η is not purely real. On the contrary, instead, the two-form describing the phase (2.68) must vanish when time reversing boundary conditions are invoked, i.e. when η is real.
We remark that the relevant group in hyperbolic geometry is $\mathrm{PSL}(2,\mathbb{R})$ the group of real Möbius transformations. The Lie algebra of this group is the space of real 2×2 traceless matrices which are spanned by σ_1, σ_3 and $i\sigma_2$, where the σs are the usual Pauli matrices. The two generators σ_3 and $\sigma_+ = \sigma_1 + i\sigma_2$ form a closed subalgebra. The structure of this Lie subalgebra is exactly the same as ours: the commutator of the virial operator and the momentum operator is the momentum operator, namely,

$$[x \circ p, p] = i\hbar p. \tag{2.71}$$

2.6 The regularization procedure: an equivalent perspective

One may object to the regularization scheme introduced in the previous section for its artificiality. In fact, in order to have a well-posed problem we embedded our original problem into a larger space, $L^2(\mathbb{R})$, and needed to make sense of the differential in (2.50). In this section we are going to

understand better what may be the problem in the definition of the derivative with respect to our parameters, and, moreover, we are going to show an alternative, intrinsic, approach to renormalization which does not make use of any embedding.
Let us consider the following map:

$$(l,c) \in \mathbb{R}_+ \times \mathbb{R} \mapsto \zeta(l,c) = U^\dagger(l,c)\zeta = V(c)\, W(\ln l)\zeta \in L^2(\mathbb{R}), \tag{2.72}$$

where $\zeta \in L^2(\mathbb{R})$ is a suitable unit vector independent of (l,c), and $U(l,c)$ is defined in (2.43). We would like to understand better the following differential:

$$(\mathrm{d}\zeta)(x) = \left(\frac{\partial}{\partial l}\zeta\right)(x)\mathrm{d}l + \left(\frac{\partial}{\partial c}\zeta\right)(x)\mathrm{d}c. \tag{2.73}$$

Fix $l > 0$ and consider the restriction of (2.72) to its second argument

$$c \in \mathbb{R} \mapsto U^\dagger(l,c)\zeta = V(c)\, W(\ln l)\zeta. \tag{2.74}$$

$\{V(c)\}_{c\in\mathbb{R}}$ in (2.40) form a one-parameter group, whose generator is the momentum p defined in (2.39). Thus,

$$\frac{\partial}{\partial c}\zeta(l,c) = \left(\frac{\mathrm{d}}{\mathrm{d}c}V(c)\right)\left(W(\ln l)\zeta\right) = -\frac{\mathrm{i}}{\hbar}\, pV(c)\left(W(\ln l)\zeta\right), \tag{2.75}$$

which is well posed if and only if $W(\ln l)\zeta \in H^1(\mathbb{R})$. For this reason we can interpret $\partial\zeta(l,c)/\partial c$ as the distributional derivative of $\zeta(l,c)$ which is forced to belong to $L^2(\mathbb{R})$. In our case the extension of the eigenfunction to the real line is smooth, $\tilde{\phi}_n(l,c) \in C^\infty(\mathbb{R})$, so that the derivatives can be computed classically. Clearly $\partial\tilde{\phi}_n(l,c)/\partial c$ is only locally summable over the real line.
Since the restriction of smooth functions to open subsets is still smooth and since from a physical perspective we can have information only on what happens on the inside of the one dimensional box, $I_{l,c}$, we give the following prescription:

$$\frac{\partial}{\partial c}\phi_n(l,c) := \frac{\partial}{\partial c}\tilde{\phi}_n(l,c)\Big|_{\mathring{I}_{l,c}} \tag{2.76}$$

being an element of $C^\infty(\mathring{I}_{l,c})$ and locally summable. An analogous prescrip-

tion works for the derivative with respect to l. Let us return to our problem settled in $L^2(I_{l,c})$. This time the one-form is given by

$$\langle\phi_n|\mathrm{d}\phi_n\rangle = \left(\int_{I_{l,c}} \overline{\phi_n(x)} \left(\frac{\partial}{\partial l}\phi_n\right)(x)\mathrm{d}x\right)\mathrm{d}l + \left(\int_{I_{l,c}} \overline{\phi_n(x)} \left(\frac{\partial}{\partial c}\phi_n\right)(x)\mathrm{d}x\right)\mathrm{d}c, \tag{2.77}$$

where the derivatives in (2.77) are to be considered in the sense stated above, that is as locally integrable functions in $\mathring{I}_{l,c}$. Once more,

$$\int_{I_{l,c}} \overline{\phi_n(x)}\frac{\partial}{\partial l}\phi_n(x)\mathrm{d}x = \int_{I_{l,c}} \frac{\partial}{\partial l}|\phi_n(x)|^2\mathrm{d}x - \int_{I_{l,c}} \phi_n(x)\frac{\partial}{\partial l}\overline{\phi_n(x)}\mathrm{d}x. \tag{2.78}$$

Due to normalization the first factor in the second member vanishes so that

$$\mathrm{Re}\left(\int_{I_{l,c}} \overline{\phi_n(x)}\frac{\partial}{\partial l}\phi_n(x)\mathrm{d}x\right) = 0, \tag{2.79}$$

while as before we get

$$\int_{I_{l,c}} \overline{\phi_n(x)}\frac{\partial}{\partial l}\phi_n(x)\mathrm{d}x = i\,\mathrm{Im}\int_{I_{l,c}} \overline{\phi_n(x)}\frac{\partial}{\partial l}\phi_n(x)\mathrm{d}x, \tag{2.80}$$

and an analogous expression for the partial derivative with respect to c holds. With this in mind we are able to get the same result (2.65) as before, by reaching the boundary from the "inside", rather than from the "outside", so that our new prescription, though equivalent to the one discussed above, may appear more natural. This is coherent from a physical perspective since we can have information only on what happens on the inside of the one dimensional box $I_{l,c}$.

2.7 The degenerate case

For completeness, we are going to investigate the exceptional cases $\eta = \pm 1$, which, as mentioned before, correspond to degenerate spectra. For $\eta = 1$ we have that for any $n \geq 1$ the two eigenvalues λ_n and λ_{-n} in (2.53) coalesce,

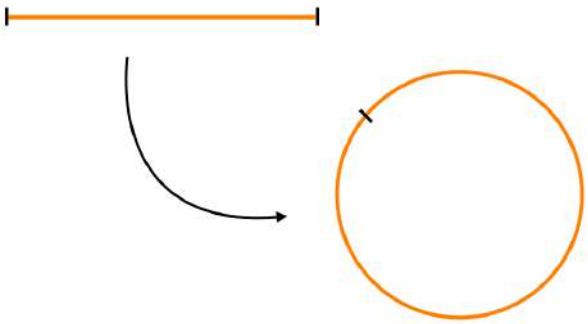

Figure 2.10: Periodic boundary conditions: the boundary's ends can be topologically identified.

and an orthonormal basis in the n-th eigenspace is given by

$$\phi_n^I(x) = \sqrt{2}\,\cos(2\pi n\,x), \qquad \phi_n^{II}(x) = \sqrt{2}\,\sin(2\pi n\,x), \qquad n \geq 1. \tag{2.81}$$

For $\eta = -1$, we have instead that $\lambda_n = \lambda_{-n-1}$, and a possible choice of an orthonormal basis is

$$\phi_n^I(x) = \sqrt{2}\,\cos((2n{+}1)\pi\,x), \qquad \phi_n^{II}(x) = \sqrt{2}\,\sin((2n{+}1)\pi\,x), \qquad n \in \mathbb{N}. \tag{2.82}$$

From the general theory of geometric phases [WZ83] it is well known that a degenerate spectral decomposition gives rise to a one-form connection in terms of a Hermitian matrix and from a geometrical perspective this corresponds to a connection on a principal bundle, whose typical fiber is identified with a non-Abelian group.
Let us consider the case $\eta = 1$, which physically corresponds to periodic boundary conditions. We need to compute the following matrix one-form:

$$\mathcal{A}^{(n)} = i \begin{pmatrix} \langle \phi_n^I | \mathrm{d}\phi_n^I \rangle & \langle \phi_n^I | \mathrm{d}\phi_n^{II} \rangle \\ \langle \phi_n^{II} | \mathrm{d}\phi_n^I \rangle & \langle \phi_n^{II} | \mathrm{d}\phi_n^{II} \rangle \end{pmatrix}, \tag{2.83}$$

where the coefficients of the differentials are to be considered in the distri-

butional sense. The former equation yields the following result:

$$\mathcal{A}^{(n)} = \mathcal{A}_l^{(n)} \mathrm{d}l + \mathcal{A}_a^{(n)} \mathrm{d}c = \frac{k_n}{l} \sigma_2 \mathrm{d}c. \tag{2.84}$$

where σ_2 is the second Pauli matrix. For a non-Abelian principal fiber bundle, the curvature two-form, according to the Cartan structure equation, is provided by

$$\mathcal{F}^{(n)} = \mathrm{d}\mathcal{A}^{(n)} + \frac{1}{2}[\mathcal{A}^{(n)}, \mathcal{A}^{(n)}]. \tag{2.85}$$

Plugging in the explicit expression of the above one-form (2.84) we find that

$$\mathcal{F}^{(n)} = \mathrm{d}\mathcal{A}^{(n)}. \tag{2.86}$$

The latter equation shows explicitly that, although every fiber is two dimensional, the overall bundle is trivial. The one-form connection in (2.84) can be *globally* diagonalized making use of the basis of plane waves. Indeed, if we had started from a "rotated" basis, instead of (2.81):

$$\phi_n^I(x) \pm \mathrm{i}\, \phi_n^{II}(x) \propto \mathrm{e}^{\pm \mathrm{i}\, \mathrm{k_n x}}, \tag{2.87}$$

due to Euler's identity, and computed (2.84) in this new basis, we would have obtained a diagonal matrix. In the most general case, instead, one is able to determine only a *local* basis where the above one-form (2.84) is diagonal. On the other hand, in our case the bundle can be globally trivialized.
The case of $\eta = \pm 1$ is exceptional since it has degeneracies in the spectrum. In this case one may expect to find a $U(2)$ non-Abelian geometric phase of the type discussed by Wilczek and Zee [WZ83]. However, we find that the phase is a diagonal subgroup of $U(2)$ and is essentially Abelian. This is easy to understand from time reversal symmetry. Since translations and dilations are real operations, they commute with time reversal and so the allowed $U(2)$ must also be real. This reduces $U(2)$ to $O(2)$, which is Abelian. By a suitable choice of basis one can render the connection diagonal as in (86). The "non-Abelian" $U(2)$ Wilczek-Zee phase is in fact in an Abelian subgroup. It is also worth noting that the approach to $\eta = \pm 1$ is a singular limit because of the

degeneracy there.
It is also interesting to note that the adiabatic transformations we consider act quite trivially on the spectrum of the Hamiltonian. Indeed, the translations are isospectral and the dilations only cause an overall change in the scale of the energy spectrum $\lambda_n \to \lambda_n/l^2$. In particular, there are no level crossings and no degeneracies (away from $\eta \neq \pm 1$). This illustrates a remark made by Berry in the conclusion of [Ber84]: although degeneracies play an important role in Berry's phase, they are not a necessary condition for the existence of geometric phase factors. Indeed, our example reiterates this point. The Berry phases are nonzero even though one of the deformations is isospectral and the other a simple scaling. It is the twisting of the eigenvectors over the parameter space that determines the Berry connection and phase, not the energy spectrum.

2.8 The physics of quantum phases

Berry's discovery unveiled some properties of quantum mechanics, which had been neglected for a very long time. Although, Dirac himself [Dir31b], and others, e.g. Aharonov and Bohm [AB59] had studied the problem of topological phases, the geometry of the adiabatic evolution had not been completely understood before Berry. Today, we are also aware that adiabatic evolution is just a technical tool, since geometric phases can arise in general cyclic evolution as shown in the work of Aharonov and Anandan [AA87], and Samuel and Bhandari [SB88].
In the present section we would like to discuss a particular experiment, done by T. Bitter and D. Dubber in 1987 [BD87], which showed incontrovertibly the existence of the Berry phase in a spin system under the influence of a cycling magnetic field.
The paradigm of geometric phases is provided by a spin one-half particle in a slowly varying magnetic field, which plays the role of the external environment. The experiment we would like to discuss involves the measurement of the polarization of a beam of neutrons after the interaction with an helical magnetic field. The resulting shift, if any, in polarization will have the

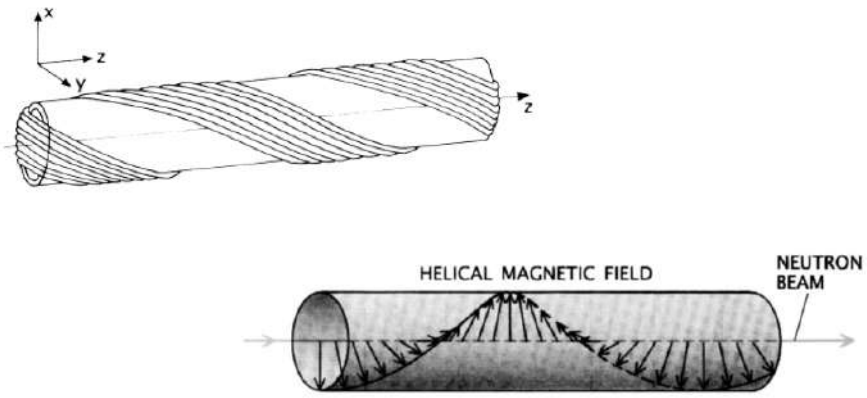

Figure 2.11: The Experiment by Bitter and Dubber.

information about the geometric phase we are looking for.
Bitter and Dubber used a brilliant experimental setup in order to unveil the Berry phase contribution to polarization. They took a beam of neutrons travelling at a speed of 500 m/s, which was polarized up to the 97%.
This high degree of polarization meant that almost all the magnetic moments associated to the neutrons were all parallel to a given direction. The beam was, then, sent through a tube where an helical magnetic field was produced by a coil wrapped onto it (Figure 2.11).
The hamiltonian for the neutrons in this experiment is thus:

$$H = \frac{\boldsymbol{p}^2}{2m} - \boldsymbol{\mu} \cdot \boldsymbol{B}. \tag{2.88}$$

where $\boldsymbol{p}$ is the neutron momentum, m its mass, while $\boldsymbol{\mu}$ its magnetic dipole moment. We can neglect gravitational or electromagnetic interactions, so that the particle trajectories do not bend, and neutrons follow their original path.
In the center of mass frame of the neutron the magnetic dipole moment interacts with a magnetic field that traces one complete revolution around the origin. In this case the angle described by the tip of the vector representing the magnetic field is exactly 2π.
In order to modify the value of this angle, an extra magnetic field coaxial to the tube could be added. Bitter and Dubbers then posed the following

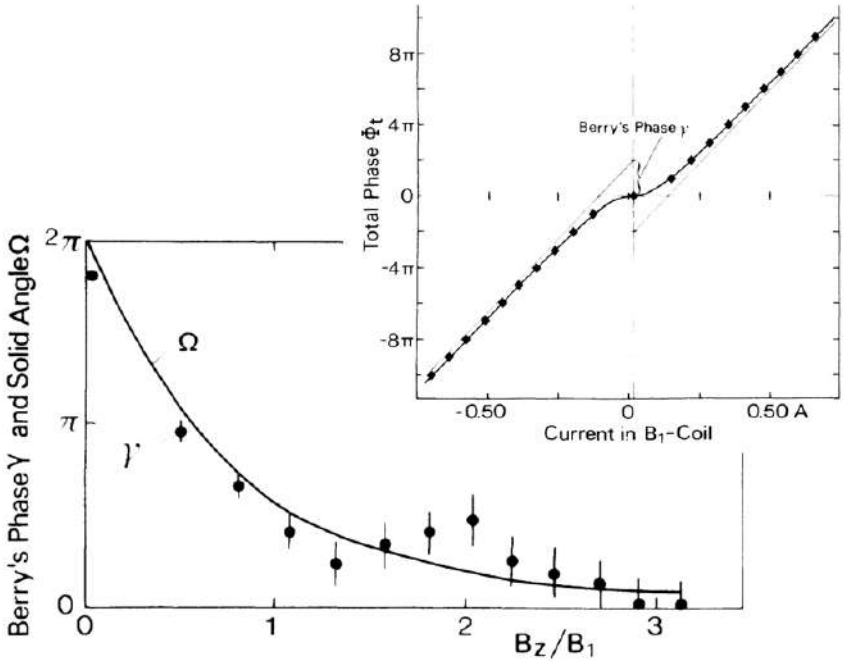

Figure 2.12: The experimental results show a good agreement between the hypothesis of the Berry phase and the data obtained.

question:"Given that the particles are injected into the tube with a certain polarization, what would be the intensity of the beam as it leaves the experimental setup and gets probed by an output analyzer?" The interesting part is that this problem can be studied exactly and the Berry phase can be computed as a limiting case. In this experimental setup the adiabatic limit corresponds to the direction of the magnetic field changing slowly compared to its amplitude, or, more precisely to the precession frequency of the spin around the field. One can prove that the total phase after a travel in the tube, in the adiabatic limit, is:

$$\phi_t = bT - 2\pi, \tag{2.89}$$

where b is the field strength times the gyromagnetic ratio of the neutrons, T is the period associated to a single turn-around. We can interpret the above formula in these terms: the first contribution represents the dynamical phase,

while the second one, which is time-independent, heavily relies on the path followed by the magnetic field. It is this latter that is interpreted as Berry's phase, whose origin is purely geometrical. In fact, if we switch on the extra magnetic field, the coaxial one, we can modify the solid angle $2\pi(1-\cos\theta)$ which is enclosed by the path, and consequently obtain different contributions as shown in (Figure 2.12).

So far we have discussed only one experimental evidence of geometric phases, probably the simplest one, which dealt with Berry's phase. Moreover in this case the environment has to be considered classical (the magnetic field) and can be manipulated by the experimenter. In more realistic cases, the environment itself could be a quantum system and geometric phases can appear in molecular systems as a result of the interaction between electronic and rotational motions or of the interaction between electronic and vibrational motions. In these cases a fictitious magnetic flux appears in the Born-Oppenheimer approximation, which, introducing gauge potential terms, gives rise to some geometric phases.

Moreover geometric phases can be associated with Bloch waves in crystalline solids and with adiabatic particle transport linked to polarization calculations for crystal dielectrics. So far, the most fascinating application of the geometric phase could be considered the already discussed quantum-Hall effect. As shown in section 1.4 it is a quantum phenomenon involving two-dimensional electron systems in strong magnetic fields and low-temperatures. In the case of the integer quantum-Hall effect, the quantization of the Hall conductance can be explained in terms of a topological invariant: the Chern number.

Furthermore the concept of geometric phase has proved to be a fundamental tool in the study of spin-wave dynamics in itinerant magnets [NK98]. Spin waves are collective modes of motion in the local magnetic moments in magnetized materials. The simplest approach to the problem is provided by the Heisenberg model, where the spins are bound to atomic sites. There are other cases where the itinerant picture is far more interesting: the spins are carried by Bloch states moving throughout the system. It is a matter of fact that the calculation of spin waves for itinerant-electron systems has been an undiscovered area in condensed matter physics. Geometric phases

have proved to be essential in order to properly understand the underlying structures.

A lot of improvements have been made so far, and geometric phases have been studied in different contexts showing unexpected and surprising results. The variety of applications shows us how fertile is the field of geometric phases and who knows what we could expect in the next near future. For a complete review on geometric phases and a detailed description of the above cited results an excellent reference is [Boh+03].

Chapter 3

Quantum cavities with alternating boundary conditions.

In this chapter we are going to take into account a dynamical situation involving quantum boundary conditions [FGL17a]. The study of time dependent boundaries offers noticeable physical perspectives ranging from atoms in cavities, to superconducting quantum interference devices (SQUID), to atoms and ions in magnetic traps and microwave cavities.
Here we are going to concentrate on a dynamical evolution à la Trotter and we are going to rapidly interchange a couple of boundary conditions. The main objective will be to understand and investigate the limiting dynamics.

3.1 Alternating boundary conditions

Let us consider a quantum particle confined into a cavity $\Omega \subset \mathbb{R}^n$, Ω being an open connected set, whose boundary $\partial\Omega$ is a smooth submanifold of $\mathbb{R}^n$. The particle in the cavity is spinless, free and has mass m.
The effective mathematical description of this system is provided by the free

Hamiltonian

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\Delta, \tag{3.1}$$

that is the the kinetic energy operator. Here Δ is the Laplacian settled on some dense subspace of $L^2(\Omega)$, the Hilbert space of square integrable functions on Ω.

We are going to denote with $\mathscr{H}_b$, which will be specified later, the Hilbert space of the wave functions' boundary values. Unfortunately the Hilbert space at the boundary, say $\mathscr{H}_b$, cannot be identified with the space of square integrable functions on the border, say $L^2(\partial\Omega)$. Indeed, it may happen that the boundary value of a function in $L^2(\Omega)$ is a distribution (see the example at the end of the Appendix).

As discussed in chapter 5 and proved in [AIM05; FGL17b] every unitary operator U acting on the Hilbert space at the boundary $\mathscr{H}_b$ uniquely determines a well defined physical realization of the Hamiltonian H, i.e a self-adjoint extension of H, denoted by H_U, identified by some boundary conditions.

The objective will be to uncover what happens when we rapidly interchange the conditions at the border.

Consider H_{U_1} and H_{U_2}, two realizations of H, corresponding to two boundary conditions, given by U_1 and U_2, unitary operators on $\mathscr{H}_b$. Moreover we let the two boundary conditions rapidly alternate. More precisely, if the boundary conditions are switched at a rate t/N, the overall unitary evolution reads

$$\begin{aligned}&\underbrace{\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)\dots\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)}_{N\text{ times}}\\ &\quad=\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)^N.\end{aligned} \tag{3.2}$$

This equation is an example of Trotter product formulas [Tro59]. Similar evolutions show up in different areas of quantum mechanics. For example they emerge in in the looming dynamics associated to the Quantum Zeno effect [FP08; FL10; GFL10] as well as they have remarkable applications in quantum chaos [Cas+79; Ber+79]. Lastly, but not less importantly, the Trotter product formula is fundamental in the definition of the Feynman

path integral [JL00].
The problem we are dealing with was originally addressed in [Aso+13]. It is a matter of interest to show whether in the $N \to +\infty$ limit, the overall evolution is unitary. From a physical point of view the $N \to +\infty$ limit means that the time interval between the switches of U_1 and U_2 goes to zero, the number of switches goes to infinite, while the total time $2t$ is kept constant. The final evolution, then, reads:

$$\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tH_W}, \quad N \to +\infty \tag{3.3}$$

in terms of a new realization of the Hamiltonian H, say H_W , with some boundary conditions specified by the boundary unitary operator W.

3.2 Trotter Formulas

The answer to the limiting dynamics problem dates back to deep mathematical results on product formulas. Trotter [Tro59] proved that for every A and B self-adjoint operators such that their sum is self-adjoint (on the intersection of their domains $D(A) \cap D(B)$), then

$$\left(\mathrm{e}^{-\mathrm{i}tA/N}\mathrm{e}^{-\mathrm{i}tB/N}\right)^N \to \mathrm{e}^{-\mathrm{i}t(A+B)}, \quad N \to +\infty. \tag{3.4}$$

Of course, one should specify the topology used for the above convergence. For further details we refer the reader to the original paper [Tro59] or the book [JL00].
Unfortunately, the intersection of the domains of two self-adjoint extensions of T is too small, and $T_{U_1} + T_{U_2}$ is not self-adjoint (not even its closure!), so that this result cannot be applied to our case.
In order to overcome this obstacle it is sufficient to take into account the quadratic forms associated to the operators (i.e. the expectation values of the observables), instead of the operators themselves. It is well known [Neu55] that

$$t_U(\psi) = \langle \psi | H_U \psi \rangle_{L^2(\Omega)} = -\frac{\hbar^2}{2m} \int_\Omega \overline{\psi(x)}\, \Delta\psi(x)\, \mathrm{d}x \tag{3.5}$$

represents the expectation value of the kinetic energy operator in the state ψ. From the mathematical point of view, t_U is the quadratic form associated to H_U, whose domain can be considerably larger than $D(H_U)$ (See chapter 5).

Starting from t_{U_1} and t_{U_2}, one can build the quadratic form $(t_{U_1} + t_{U_2})/2$ defined on the (dense) intersection of the respective domains $D(t_{U_1})$ and $D(t_{U_2})$, namely $D = D(t_{U_1}) \cap D(t_{U_2})$.

It can be proved [Kat66], that there is one and only one self-adjoint operator, denoted by $H_{U_1} \dot{+} H_{U_2}$ and called the form sum operator of H_{U_1} and H_{U_2}, corresponding to the form $t_{U_1} + t_{U_2}$, i.e. such that

$$t_{H_{U_1} \dot{+} H_{U_2}} = t_{H_{U_1}} + t_{H_{U_2}}. \tag{3.6}$$

This idea, introduced by Kato [Tro78], was elaborated by Lapidus et al. [Lap82; ENZ11] who found the ultimate version of the Trotter product formula

$$\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)^N \to \mathrm{e}^{-\mathrm{i}t(H_{U_1} \dot{+} H_{U_2})}, \quad N \to +\infty. \tag{3.7}$$

when H_{U_1} and H_{U_2} are bounded from below. As a technical remark notice that, as a consequence of the weakening of the hypotheses, the convergence of the product formula when the operator sum is not self-adjoint is in a weaker topology than in Trotter's case; more precisely equation (3.4) holds pointwise, namely

$$\lim_{N\to+\infty} \left(\mathrm{e}^{-\mathrm{i}tA/N}\mathrm{e}^{-\mathrm{i}tB/N}\right)^N \psi = \mathrm{e}^{-\mathrm{i}t(A+B)}\psi, \quad \text{for all } \psi \in L^2(\Omega), \tag{3.8}$$

while its weaker counterpart (3.7) is valid only on average [ENZ11], that is to say

$$\lim_{N\to\infty} \int_{\mathbb{R}} \left[\left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)^N \psi - \mathrm{e}^{-\mathrm{i}t(H_{U_1} \dot{+} H_{U_2})}\psi\right] f(t)\,\mathrm{d}t = 0 \tag{3.9}$$

for all $\psi \in L^2(\Omega)$ and for all $f \in \mathscr{D}(\mathbb{R})$, the space of test functions in $\mathbb{R}$, that is the space of compactly supported and smooth functions on $\mathbb{R}$. The validity of the above formula in a stronger topology is still a matter of debate

as pointed out in [Lap82; ENZ11].

3.3 A composition law of boundary conditions: a first glimpse

In the analysis of the dynamics of boundary conditions we are considering one of the paradigmatic examples in nonrelativistic quantum mechanics, that is, the case of a free particle confined in a cavity Ω in the space $\mathbb{R}^n$.
As already mentioned, the cavity is going to be subjected to a rapid switching between two different boundary conditions. We are going to show that the emerging dynamics, in the limit of infinitely frequent switchings, yields new boundary conditions combining the initial ones in an appropriate sense. Up to what explained until this point we have that

$$\lim_{N\to+\infty} \left(\mathrm{e}^{-\mathrm{i}tH_{U_1}/N}\mathrm{e}^{-\mathrm{i}tH_{U_2}/N}\right)^N = \mathrm{e}^{-\mathrm{i}2tH_W}, \tag{3.10}$$

where

$$H_W = \frac{H_{U_1} \dot{+} H_{U_2}}{2}. \tag{3.11}$$

In the next sections we are going to prove that H_W is a new realization of the operator H with new boundary conditions specified by a unitary operator W obtained combining U_1 and U_2 in a suitable way.
The operator W is the following

$$W = U_1 * U_2 := P_W + \mathscr{C}\left(\frac{\mathscr{C}^{-1}(V_{U_1})Q_{U_1} + \mathscr{C}^{-1}(V_{U_2})Q_{U_2}}{2}\right) Q_W, \tag{3.12}$$

where:

- $Q_W = Q_{U_1} \wedge Q_{U_2}$ is the projection onto the intersection of the ranges of Q_{U_1} and Q_{U_2}, and $P_W = I - Q_W$ is the spectral projection of W onto the eigenspace with eigenvalue 1;
- every U_i $(i = 1, 2)$ can be uniquely decomposed in the sum $P_{U_i} + V_{U_i}$, where P_{U_i} is the spectral projection of U_i on the eigenspace with

eigenvalue 1, $Q_{U_i} = I - P_{U_i}$, and $V_{U_i} = Q_{U_i} U_i Q_{U_i}$ is the projection of U_i on the range of Q_{U_i};

- with the symbols $\mathscr{C}$ and $\mathscr{C}^{-1}$ we denote, respectively, the Cayley transform and its inverse. As recalled in section 5.8 the Cayley transform maps the set of self-adjoint operators onto the set of unitary operators which do not have 1 as an eigenvalue. Indeed, for every self-adjoint operator A on a Hilbert space, the operator

$$\mathscr{C}(A) = (A - \mathrm{i}I)(A + \mathrm{i}I)^{-1}, \tag{3.13}$$

is unitary. Conversely, for every unitary operator V such that $I - V$ is invertible, the operator

$$\mathscr{C}^{-1}(V) = \mathrm{i}\,(I + V)(I - V)^{-1}, \tag{3.14}$$

is self-adjoint on the range of $(I - V)$.

3.4 The one dimensional case

Before delving into the study of the composition law for boundary conditions in $\Omega \subset \mathbb{R}^n$, we would like to express the results discussed in [Aso+13] in a more general framework, suitable for a quick generalization to higher dimensions.
We start by considering a particle confined in an interval $\Omega = (0, 1)$ of the real line. In this case the Hamiltonian associated to the free quantum particle is the one-dimensional Laplacian:

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{3.15}$$

acting on some dense space of $L^2(0, 1)$. Remarkably, in the one-dimensional case, the boundary $\partial\Omega = \{0, 1\}$ contains only two points and the Hilbert space of the boundary values is two dimensional, that is $\mathscr{H}_b = L^2(\{0, 1\})\mathbb{C}^2$. As proved in [AIM05], the whole family of self-adjoint extensions of H is in

a one-to-one correspondence with the possible boundary conditions coming out from U(2), the set of 2×2 unitary matrices. More precisely, to each $U \in \mathrm{U}(2)$ corresponds a unique self-adjoint extension

$$H_U = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{3.16}$$

acting on the domain

$$D(H_U) = \{\psi \in H^2(0,1) : \ \mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}\}, \tag{3.17}$$

where φ and $\dot{\varphi}$ are the boundary data of the wave function ψ and are defined as

$$\varphi := \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix}, \qquad \dot{\varphi} := \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix}. \tag{3.18}$$

We recall that $H^2(0,1)$ is the Sobolev space of square integrable functions ψ with square integrable first and second derivative, respectively ψ' and ψ'' [AF02; Bre10].

Moreover any wave function ψ in the domain of H_U satisfies the boundary conditions

$$\mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}. \tag{3.19}$$

This parametrization of the self-adjoint extensions of H in terms of unitary operators on the boundary differs lightly from the one presented in [Aso+13], nevertheless, the two parametrizations are equivalent.

Next, we are going to show how the equation of boundary conditions (3.19) is related to the eigenprojection with eigenvalue 1 in the spectrum of U, from now on denoted by P_U. The orthogonal projector will be denoted by Q_U, such that $Q_U + P_U = I$. Notice that P_U can degenerate into the identity when $U = I$, as well as it can be the zero operator when 1 is not an eigenvalue of U.

By means of P_U and Q_U we are able to recast U in equation eq:bc2 into a

sum on orthogonal eigenspaces, that is:

$$U = P_U + V_U, \tag{3.20}$$

$$V_U = UQ_U = Q_U U = Q_U\, U\, Q_U. \tag{3.21}$$

Notice that the operator V_U is unitary on the range of Q_U and 1 does not belong to its spectrum.
Having this decomposition at hand, we can give an equivalent characterization of the domain of H_U by projecting equation (3.19) onto the range of P_U and Q_U:

$$\mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi} \quad \Longleftrightarrow \quad \begin{cases} P_U\,\varphi = 0, \\ Q_U\dot{\varphi} = -K_U\varphi, \end{cases} \tag{3.22}$$

where K_U is (minus) the inverse Cayley transform of V_U, that is

$$K_U = -\mathscr{C}^{-1}(V_U)Q_U = -\mathrm{i}\,(I+V_U)(I-V_U)^{-1}Q_U, \tag{3.23}$$

where $(I-V_U)^{-1}$ makes perfectly sense, since 1 is not an eigenvalue of V_U. Equation (3.22) is valid for every unitary U, and it particularizes to special forms according to the expression of the spectral projection P_U. We can distinguish among three cases:

a) 1 is a double degenerate eigenvalue of U, therefore $P_U = I$. This corresponds to Dirichlet boundary conditions;

b) 1 is a non degenerate eigenvalue of U, therefore $U = P_U + \lambda\, Q_U$, with $|\lambda| = 1$ and $\lambda \neq 1$. This case corresponds to: $Q_U\dot{\varphi} = \mathrm{i}\,(1+\lambda)(1-\lambda)^{-1}\, Q_U\varphi\,,\ P_U\varphi = 0$;

c) 1 is not an eigenvalue of U, therefore $P_U = 0$. For example if $U = -I$, we find Neumann boundary conditions, which are a particular case of Robin boundary conditions. The latter can be found, for example, when

$$U = \begin{pmatrix} -\mathrm{e}^{\mathrm{i}\alpha_1} & 0 \\ 0 & -\mathrm{e}^{\mathrm{i}\alpha_2} \end{pmatrix}, \tag{3.24}$$

with $\alpha_1, \alpha_2 \in (-\pi, \pi)$, and

$$\psi'(0) = \tan\frac{\alpha_1}{2}\,\psi(0), \qquad \psi'(1) = -\tan\frac{\alpha_2}{2}\,\psi(1). \tag{3.25}$$

Summing up: case a) happens when $U = I$, which corresponds to a constraint on both the values of the wave function at the boundary. Case b) provides, instead, a constraint only on one value of the wave function at the boundary. For example, when $U = P_U - \mathrm{e}^{\mathrm{i}\alpha}Q_U$, with $\alpha \in (-\pi, \pi)$ and P_U being the projection onto the span of $(1, 0)$ we obtain:

$$\psi(0) = 0 \qquad \psi'(1) = -\tan\frac{\alpha}{2}\,\psi(1). \tag{3.26}$$

Eventually, when 1 is not an eigenvalue, no constraint on the value at the border arises from case c). It is clear now how the behavior of the wave functions at the border is interwisted with the presence of the eigenvalue 1 in the spectrum of U.

3.4.1 Quadratic forms

In this subsection we analyze the relation between a self-adjoint operator H_U and its associated quadratic form t_U. First of all we will explain how to get the form t_U from the operator H_U and then we will show how to go in the opposite way.

Let H_U be a self-adjoint extension related to the unitary matrix $U \in \mathrm{U}(2)$ and we study the associated quadratic form t_U. An integration by parts yields the following result:

$$\begin{aligned} t_U(\psi) &= \langle\psi \mid H_U\psi\rangle_{L^2(\Omega)} = -\frac{\hbar^2}{2m}\int_0^1 \overline{\psi(x)}\,\psi''(x)\,\mathrm{d}x \\ &= \frac{\hbar^2}{2m}\int_0^1 |\psi'(x)|^2\,\mathrm{d}x - \overline{\psi(1)}\,\psi'(1) + \overline{\psi(0)}\,\psi'(0) \\ &= \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} - \langle\varphi|\dot\varphi\rangle_{\mathbb{C}^2}\right), \quad \text{for all } \psi \in D(H_U), \end{aligned} \tag{3.27}$$

where φ and $\dot\varphi$ are the boundary data in equation (3.18), and $\langle\alpha|\beta\rangle_{\mathbb{C}^2} =$

$\overline{\alpha}_1\beta_1+\overline{\alpha}_2\beta_2$ is the canonical scalar product in $\mathbb{C}^2$. Therefore, the expectation value of the kinetic energy of the particle has both contributions from the bulk and from the boundary.
Making use of the boundary conditions in H_U given by Eq. (3.19), we can express the former quadratic form in a more convenient fashion by trading the boundary values of the derivative for the boundary values of the function. Indeed, one gets:

$$\langle\varphi|\dot{\varphi}\rangle_{\mathbb{C}^2} = \langle(P_U+Q_U)\varphi|\dot{\varphi}\rangle_{\mathbb{C}^2} = \langle\varphi|Q_U\dot{\varphi}\rangle_{\mathbb{C}^2} = -\langle\varphi|K_U\varphi\rangle_{\mathbb{C}^2}, \tag{3.28}$$

whence

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K_U\varphi\rangle_{\mathbb{C}^2}\right), \quad \text{for all } \psi\in D(H_U). \tag{3.29}$$

Therefore, since $D(H_U)$ is a core for $D(t_U)$, the form domain $D(t_U)$ is given by

$$D(t_U) = \{\psi\in H^1(0,1)\,:\,P_U\varphi = 0\}, \tag{3.30}$$

where, $H^1(0,1)$ is the Sobolev space of square integrable functions with square integrable first derivative [AF02; Bre10]. The quadratic form t_U is closed and bounded from below, namely

$$t_U(\psi) \geq -C\|\psi\|^2_{L^2(0,1)}, \quad \text{for all } \psi\in D(t_U), \tag{3.31}$$

for some constant C depending on the norm $\|K_U\| < +\infty$ and on the continuity of the restriction map to the border

$$\psi\in H^1(0,1)\mapsto\varphi = \psi|_{\partial\Omega} = \begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix}\in\mathbb{C}^2. \tag{3.32}$$

Therefore the quadratic form t_U associated to a generic self-adjoint extension H_U of H has the following properties:

- the value of the form in the wave function ψ is given by two terms

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K_U\varphi\rangle_{\mathbb{C}^2}\right), \tag{3.33}$$

the first one is common to all the extensions while the second one depends explicitly on the extension. Notice, in fact, that the matrix K_U is, up to a sign, the inverse Cayley transform of the unitary matrix U with the eigenvalue 1 stripped out.

- the form domain $D(t_U)$ is expressed in terms of P_U, the eigenprojection with eigenvalue 1 of the unitary matrix U which identifies the extension H_U:

$$D(t_U) = \{\psi \in H^1(0,1) \,:\, P_U\varphi = 0\}; \tag{3.34}$$

- the form t_U is closed and bounded from below and its lower bound depends on the norm of the self-adjoint matrix K_U and by the continuity of the restriction map defined in (3.32):

Next, we are going to explain how to obtain the self-adjoint operator from the quadratic form. We consider a quadratic form t having the same properties explained above, namely such that

$$t(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K\varphi\rangle_{\mathbb{C}^2}\right), \qquad D(t) = \{\psi \in H^1(0,1) \,:\, P\varphi = 0\}, \tag{3.35}$$

where $K = K^\dagger$ is a self-adjoint matrix and P an orthogonal projection, such that $KP = PK = 0$.
It is easy to see that the form t is closed and bounded from below. There is a one-to-one correspondence between the set of closed and bounded from below quadratic forms and the set of lower bounded self-adjoint operators [Kat66], known as representation theorem. Using this correspondence one can immediately recover the self-adjoint extension H_U of H associated with the form t:

$$D(H_U) = \{\psi \in H^2(0,1) :\, \mathrm{i}(I+U)\varphi = (I-U)\dot{\varphi}\} \tag{3.36}$$

where the unitary matrix U is given by

$$U = P - \mathscr{C}(K)Q, \tag{3.37}$$

where $Q = I - P$ and $\mathscr{C}$ is the Cayley transform defined in (3.13). Notice that P is the eigenprojection of U with eigenvalue 1 and that Q is its orthogonal projection.

3.5 Composition law of boundary conditions in one dimension

We now evaluate the limit of the alternating dynamics (3.3). As already discussed, the product formula (3.3) holds with the form sum $H_W = \frac{1}{2}\left(H_{U_1} \dot{+} H_{U_2}\right)$. Thus, the evaluation of the emergent dynamics in (3.3) requires the computation of the sum

$$\begin{aligned} t_{12}(\psi) &= \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K_{12}\varphi\rangle_{\mathbb{C}^2}\right), \\ K_{12} &= \frac{1}{2}\left(K_{U_1} + K_{U_2}\right), \end{aligned} \tag{3.38}$$

where the form domain reads:

$$D(t_{12}) = D(t_{U_1}) \cap D(t_{U_2}) = \{\psi \in H^1(0,1) \,:\, P_{U_1}\varphi = 0 = P_{U_2}\varphi\}. \tag{3.39}$$

Notice that K_{12} is a self-adjoint matrix, since both K_{U_1} and K_{U_2} are. Let $Q_{12} = Q_{U_1} \wedge Q_{U_2}$, be the orthogonal projector onto the intersection of the ranges of Q_{U_1} and Q_{U_2}:

$$\mathrm{Ran}(Q_{12}) = \mathrm{Ran}(Q_{U_1}) \cap \mathrm{Ran}(Q_{U_2}). \tag{3.40}$$

Moreover define

$$P_{12} = I - Q_{12}. \tag{3.41}$$

Then, the form domain of t_{12} can be written in terms of the orthogonal projection P_{12} as:

$$D(t_{12}) = \{\psi \in H^1(0,1) \,:\, P_{12}\,\varphi = 0\}, \tag{3.42}$$

since

$$N(P_{12}) = \mathrm{Ran}(Q_{12}) = N(P_{U_1}) \cap N(P_{U_2}). \tag{3.43}$$

We recall that for a generic linear operator A, the kernel of A is $N(A) = \{\psi \in D(A) : A\psi = 0\}$, the set of zeros of the operator A.
Since t_{12} is closed and bounded from below, by means of representation theorems [Kat66], there is a unique (bounded from below) self-adjoint operator H_W such that:

$$D(H_W) = \{\psi \in H^2(0,1) \,:\, \mathrm{i}(I+W)\varphi = (I-W)\dot{\varphi}\} \tag{3.44}$$

$$t_{12}(\psi) = \langle \psi, T_W \psi \rangle \qquad \text{for all } \psi \in D(H_U). \tag{3.45}$$

where the unitary matrix $W \in \mathrm{U}(2)$ is given by

$$W = P_{12} - \mathscr{C}(K_{12})\, Q_{12}, \tag{3.46}$$

and $\mathscr{C}(K_{12})$ is the Cayley transform of K_{12} on the range of Q_{12}. Since P_{12} is the eigenprojection of W with eigenvalue 1, in accordance with our convention we have that $P_{12} = P_W$, $Q_{12} = Q_W$ and $K_{12} = K_W$. Notice that

$$K_{U_i} = -\mathscr{C}^{-1}(V_{U_i}) Q_{U_i}, \quad i = 1, 2, \tag{3.47}$$

thus we obtain that (3.46) is exactly the formula (3.12) in the one-dimensional case.

3.5.1 Examples

For the sake of concreteness let us analyze some examples for the one-dimensional case. Preliminarly, we recall that every unitary matrix $U_i, i = 1, 2$, which defines a self-adjoint extension of H can be decomposed into:

$$U_i = P_{U_i} + V_{U_i}, \tag{3.48}$$

$$V_{U_i} = Q_{U_i}\, U_i\, Q_{U_i}. \tag{3.49}$$

where P_{U_i} is the projection on the subspace with eigenvalue 1 and $Q_{U_i} = I - P_{U_i}$ and that, the self-adjoint maxtrix K_{U_i}, which appears in the boundary conditions, reads: $K_{U_i} = -\mathscr{C}^{-1}(V_{U_i})Q_{U_i}$.

- If the point 1 is not an eigenvalue for both U_1 and U_2 we have that the corresponding W matrix, encoding the boundary conditions reads:

$$W = \frac{1}{2}\mathscr{C}\left(i\frac{I+V_1}{I-V_1} + i\frac{I+V_2}{I-V_2}\right) = \frac{\frac{1}{2}\left(\frac{I+V_1}{I-V_1} + \frac{I+V_2}{I-V_2}\right) - I}{\frac{1}{2}\left(\frac{I+V_1}{I-V_1} + \frac{I+V_2}{I-V_2}\right) + I}. \tag{3.50}$$

- If 1 is a non degenerate eigenvalue for U_1 and is not an eigenvalue for U_2, then the limiting dynamics is determined by :

$$W = P_W + \frac{1}{2}\mathscr{C}\left(i\frac{I+\lambda}{I-\lambda} + i\frac{I+V_2}{I-V_2}\right)Q_W, \tag{3.51}$$

  where $P_W = P_1$ and $V_1 = \lambda Q_1$, $\lambda \in \mathbb{C}, |\lambda| = 1$.

- If 1 is a non degenerate eigenvalue for both U_1 and U_2, then:

$$W = P_W + \frac{1}{2}\mathscr{C}\left(i\frac{I+\lambda_1}{I-\lambda_1}Q_1 + i\frac{I+\lambda_2}{I-\lambda_2}Q_2\right)Q_W \tag{3.52}$$

  where $\mathrm{Ran}(Q_W) = \mathrm{Ran}(Q_{U_1}) \cap \mathrm{Ran}(Q_{U_2})$., $V_i = \lambda_i Q_i, \lambda_i \in \mathbb{C}, |\lambda_i| = 1$, for $i = 1, 2$. Since Q_1 and Q_2 are one dimensional projections it may happen that:

  - $Q_1 = Q_2$, then:

$$W = P_1 + \frac{1}{2}\mathscr{C}\left(i\frac{I+\lambda_1}{I-\lambda_1} + i\frac{I+\lambda_2}{I-\lambda_2}\right)Q_1 \tag{3.53}$$

  - $Q_1 \neq Q_2$, then $Q_W = 0$ and $W = I$. In this case we obtain Dirichlet boundary conditions.

- If 1 is a double degenerate eigenvalue for U_1, then $Q_W = 0$ and thus the resulting dynamics is encoded by Dirichlet boundary conditions.

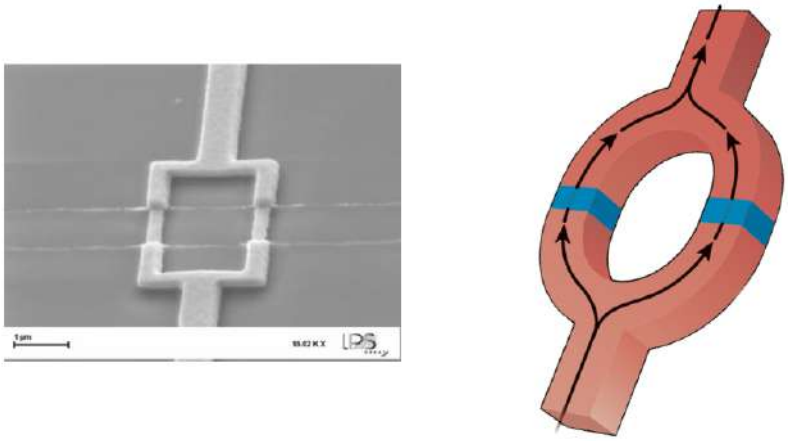

Figure 3.1: A conventional SQUID consists of a ring of superconducting material split by two barriers (in blue). The current flowing in the loop tunnels through the barrier. On the left a real SQUID circuit (Groupe Physique Mesoscopique, LPS, Orsay).

3.5.2 Physical implementation

As discussed in the previous section the limiting dynamics is described in terms of a unitary matrix $W = U_1 * U_2$, obtained by rapidly changing boundary conditions U_1 and U_2.

Moreover we have seen how starting from general boundary conditions for which 1 is a non degenerate eigenvalue and $Q_{U_1} \neq Q_{U_2}$, we obtain Dirichlet boundary conditions in the limiting dynamics.

For example one could consider pseudo-periodic boundary conditions for both U_1 and U_2:

$$U_1 = \begin{pmatrix} 0 & -\mathrm{e}^{-\mathrm{i}\alpha_1} \\ -\mathrm{e}^{\mathrm{i}\alpha_1} & 0 \end{pmatrix} \qquad U_2 = \begin{pmatrix} 0 & -\mathrm{e}^{-\mathrm{i}\alpha_2} \\ -\mathrm{e}^{\mathrm{i}\alpha_2} & 0 \end{pmatrix} \tag{3.54}$$

then the limiting dynamics, as proved in the previous section, is determined by $W = I$, which means Dirichlet boundary conditions.

This could be experimentally implemented by means of a SQUID and Josephson junctions. A SQUID (Superconducting Quantum Interference Device) is

a superconducting loop with Josephson junctions (See Figure 3.1).
Josephson [Jos62] predicted an effect which appears when two superconductors are coupled by a weak link or a tunneling junction. In particular, a Josephson junction is based on the tunneling of Cooper pairs. Interestingly the current passing through a Josephson junction acquires a phase, which can be detected in interpherometry experiments.
In particular, when arranged into a superconducting loop, the phase generated by the junctions can be varied accordingly to a magnetic field threading the loop. These effects can be used in order to simulate boundary conditions in correspondence of the junctions.
Indeed, by means of a SQUID circuit one can pulse the properties of the Josephson junction in order to simulate a Trotter-like evolution. Thus starting with pseudo-periodic boundary conditions in the junctions, then the final result will be a complete blockage of the electrical current through the circuit, namely Dirichlet boundary conditions at the junctions.

3.6 The path to higher dimensions

Here we first sum up the main steps of the construction of the composition law of boundary conditions in the one-dimensional case, i.e. $\Omega = (0,1)$ and then we introduce the main ideas to extend the result to the general n-dimensional case.

(i) First of all we have introduced the Hilbert space of boundary values $\mathscr{H}_b = \mathbb{C}^2$, then we have defined the boundary data

$$\psi \in L^2(0,1) \mapsto (\varphi, \dot{\varphi}) \in \mathscr{H}_b \times \mathscr{H}_b \tag{3.55}$$

$$\varphi = \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} \quad \dot{\varphi} = \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix} \tag{3.56}$$

of a wave function and finally we have recalled the one-to-one correspondence between unitary operators acting on $\mathscr{H}_b$ and the self-adjoint extensions of H (see Section 1.6)

(ii) We have shown that the quadratic form associated with each self-adjoint extension of H is given by the sum of two terms

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K_U\varphi\rangle_{\mathbb{C}^2}\right), \tag{3.57}$$

the first one being independent on the extension and the second one depending on the extension through the self-adjoint matrix $K_U = -\mathscr{C}^{-1}(V_U)Q_U$. The form domain $D(t_U)$ is expressed in terms of the eigenprojection P_U with eigenvalue 1 of the unitary matrix U specifying the extension:

$$D(t_U) = \{\psi \in H^1(0,1) \,:\, P_U\varphi = 0\}. \tag{3.58}$$

Moreover the form t_U is closed and bounded from below and its lower bound is related to the norm of K_U and to the continuity of the restriction map defined in (3.32):

Conversely, given a quadratic form t with all the above properties, i.e.

$$t(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K\varphi\rangle_{\mathbb{C}^2}\right), \tag{3.59}$$

with K self-adjoint matrix, on the domain

$$D(t) = \{\psi \in H^1(0,1) \,:\, P\varphi = 0\}, \tag{3.60}$$

with P orthogonal projection, $KP = PK = 0$. We have shown how to associate a self-adjoint extension of H using the representation theorem, [Kat66]. More precisely we have seen how to obtain the unitary matrix U in terms of the orthogonal projection P and of the self-adjoint matrix K:

$$U = P - \mathscr{C}(K)Q, \quad Q = I - P. \tag{3.61}$$

(iii) Finally we have considered two different self-adjoint extensions of H, say H_{U_1} and H_{U_2}, with $U_1, U_2 \in \mathrm{U}(2)$, and we have evaluated the limit of the alternating dynamics (3.3). We have studied the quadratic form

$t_{12} = \frac{1}{2}(t_{U_1} + t_{U_2})$ and we have shown that it is given by the sum of two terms

$$t_{12}(\psi) = \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{\hbar^2}{2m}\left(\|\psi'\|^2_{L^2(0,1)} + \langle\varphi|K_{12}\varphi\rangle_{\mathbb{C}^2}\right), \quad (3.62)$$

where

$$K_{12} = \frac{1}{2}\left(K_{U_1} + K_{U_2}\right), \quad (3.63)$$

on the domain

$$D(t_{12}) = \{\psi \in H^1(0,1) \,:\, P_{12}\,\varphi = 0\}. \quad (3.64)$$

The form domain $D(t_{12})$ is expressed in terms of an orthogonal projection P_{12} (defined by the equation $\mathrm{Ran}(P_{12}) = \overline{\mathrm{Ran}(P_{U_1}) + \mathrm{Ran}(P_{U_2})}$), therefore the unique self-adjoint operator H_W associated to t_{12} is specified by the unitary matrix W obtained by a composition of U_1 and U_2:

$$W = U_1 * U_2 = P_{12} - \mathscr{C}(K_{12})Q_{12} \quad (3.65)$$

with $Q_{12} = I - P_{12}$. The operator W is the result of a composition law between U_1 and U_2.

Now we retrace this procedure and we explain step by step the strategy to extend it to the general n-dimensional case, i.e. $\Omega \subset \mathbb{R}^n$.

- The first difficulty is the definition of the boundary data

$$\psi \in L^2(\Omega) \mapsto (\varphi, \dot{\varphi}) \in \mathscr{H}_b \times \mathscr{H}_b, \quad (3.66)$$

and the identification of the Hilbert space of boundary values $\mathscr{H}_b$. Once these aspects are clarified, the one-to-one correspondence between the unitary operators acting on $\mathscr{H}_b$ and the self-adjoint extensions of the operator H will hold as well as in the one-dimensional case, [FGL17b].

- Given $U \in \mathrm{U}(\mathscr{H}_\mathrm{b})$, the space of unitary operators on $\mathscr{H}_b$, we will study the quadratic form t_U associated to H_U. Mimicking the one-

dimensional case we will find that t_U is given by

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_U\varphi\rangle_{\mathscr{H}_{\mathrm{b}}}\right), \tag{3.67}$$

where ψ_{D} is the "regular component" of ψ, while K_U is a self-adjoint operator defined by

$$K_U = -\mathscr{C}^{-1}(V_U)Q_U, \quad Q_U = I - P_U, \quad V_U = Q_U U Q_U, \tag{3.68}$$

and P_U is the eigenprojection of U with eigenvalue 1. Understanding the meaning of ψ_{D} is one of the main difficulties in the study of the quadratic form t_U. A further complication arises from the fact that, in the n-dimensional case, the operator K_U can be unbounded. This means that the form t_U is not, in general, bounded from below. In order to avoid this possibility, we will consider only unitary operators $U \in \mathrm{U}(\mathscr{H}_{\mathrm{b}})$ having a spectrum with a gap around the point 1: this condition ensures that K_U is bounded.

- Finally we will extend the composition law for boundary conditions assuming that the spectra of $U_1, U_2 \in \mathrm{U}(\mathscr{H}_{\mathrm{b}})$ are both gapped around the point 1. This compatibility condition is necessary to extend the construction of the composition $U_1 * U_2$ to the n-dimensional case because it ensures that the form t_{12} is densely defined, closed and bounded from below and allows us to identify the self-adjoint extension corresponding to t_{12}.

3.7 Alternating dynamics for a particle in a cavity

In this section we are going to prove a composition law for boundary conditions in a more general framework. Rather than confining our attention to a particle on a segment, we are going to consider a particle in a cavity Ω, namely an open subset of $\mathbb{R}^n$.

Let Ω be an open bounded set in $\mathbb{R}^n$, whose boundary is regular. We are going to denote by ν be the normal to $\partial\Omega$, by convention ν is oriented towards the exterior of Ω. We define for a regular function ψ its normal derivative along ν:

$$\partial_\nu \psi = \nu \cdot (\nabla \psi)\,|_{\partial\Omega}, \tag{3.69}$$

where $\cdot$ is the scalar product of $\mathbb{R}^n$. Notice that, by definition, $\partial_\nu\psi$ is a function settled on $\partial\Omega$.

The kinetic energy for a quantum free particle in Ω is:

$$H = -\frac{\hbar^2}{2m}\Delta, \tag{3.70}$$

defined on some dense subset of $L^2(\Omega)$, for example $\mathscr{D}(\Omega)$, the space of test functions in Ω (compactly supported and smooth functions in Ω). Wave functions on this space are not able to provide information about the border because for every $\psi \in \mathscr{D}(\Omega)$: $\psi|_{\partial\Omega} = \partial_\nu\psi = 0$.

As usual we are going to denote with H^* be the adjoint operator of H defined in $D(H^*) = \{\psi \in L^2(\Omega) : -\Delta\psi \in L^2(\Omega)\}$.

We are going to identify the Hilbert space of the boundary values $\mathscr{H}_b$. It can be proved, [LM72], that the "restriction" to the border $\partial\Omega$ of a wave function $\psi \in L^2(\Omega)$, which we denoted by $\psi|_{\partial\Omega}$, belongs to $H^{-\frac{1}{2}}(\partial\Omega)$, the fractional Sobolev space of order $-1/2$. Notice that by restriction of a square integrable function we mean its trace on the border. Therefore in the n-dimensional case the Hilbert space of boundary values $\mathscr{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$ is infinite dimensional, unlike the one-dimensional case.

We are now ready to state the following result about the self-adjoint extensions of H. We briefly recall a result proved in [FGL17b] and references therein, as it will be discussed in chapter 5 that:

Theorem 1. *The set of all self-adjoint extensions of H is*

$$\left\{H_U : D(H_U) \to L^2(\Omega) |\, U \in \mathrm{U}(\mathscr{H}_\mathrm{b})\right\}, \tag{3.70}$$

where for all $U \in \mathrm{U}(\mathscr{H}_\mathrm{b})$

$$D(H_U) = \{\psi \in D(H^*) : \, i(I+U)\varphi = (I-U)\,\dot{\varphi}\,\}\,, \tag{3.70}$$

where the boundary data $(\varphi, \dot{\varphi})$ *are specified in Eq. (3.74).*

In the one-dimensional case, equation (3.19) provided a thorough parametrization of the self-adjoint extensions of the operator H. Theorem 5 states that Equation (3.19) is still valid for a general $\Omega \subset \mathbb{R}^n$ through a suitable reinterpretation of the boundary data $(\varphi, \dot{\varphi})$. In what follows we would like to provide the reader with explanations about the boundary data $(\varphi, \dot{\varphi})$. For further details we refer to chapter 5.
As discussed above, the restriction $\psi|_{\partial\Omega}$ of a wave function $\psi \in L^2(\Omega)$ to the border $\partial\Omega$ belongs to $\mathscr{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$, while its normal derivative $\partial_\nu\psi$ belongs to a different space (more precisely $\partial_\nu\psi$ belongs to $H^{-\frac{3}{2}}(\partial\Omega)$), [LM72].
For this reason equation (3.19) cannot hold by naively interpreting the boundary data $(\varphi, \dot{\varphi})$ as the pair $(\psi|_{\partial\Omega}, \partial_\nu\psi)$. Indeed, the elements of the pair are settled on different Hilbert spaces and the existence of an operator U acting both on $\psi|_{\partial\Omega}$ and $\partial_\nu\psi$ becomes meaningless. Moreover, the boundary values $\psi|_{\partial\Omega}$ and $\partial_\nu\psi$ are *not* independent data, as discussed in the Appendix, and one can show that only the normal derivative of a "regular" component ψ_D of ψ is independent of $\psi|_{\partial\Omega}$.
In order to define the regular component ψ_D of ψ, we need a useful decomposition of the domain of the adjoint $D(H^*)$:

$$D(H^*) = D(H_\mathrm{D}) + N(H^*), \qquad \psi = \psi_D + \psi_0, \tag{3.71}$$

where H_D is the self-adjoint extension of H with Dirichlet boundary conditions, that is on the domain

$$D(H_\mathrm{D}) = \{\psi \in H^2(\Omega) : \psi|_{\partial\Omega} = 0\}, \tag{3.72}$$

and

$$N(H^*) = \{\psi \in D(H^*) : -\Delta\psi = 0\} \tag{3.73}$$

is the kernel of H^*. In other words, every $\psi \in D(H^*)$ can be uniquely decomposed in the sum $\psi_{\rm D} + \psi_0$, where $\psi_{\rm D} \in D(H_{\rm D})$ is a function vanishing on the boundary, $\psi_{\rm D}|_{\partial\Omega} = 0$, and ψ_0 is a harmonic function, $-\Delta\psi_0 = 0$. See the Appendix for more details.
We are finally in the right position to define the boundary data $(\varphi, \dot\varphi)$ of a wave function $\psi \in D(T^\dagger)$:

$$\varphi = \psi|_{\partial\Omega} = \psi_0|_{\partial\Omega}, \qquad \dot\varphi = \Lambda\, \partial_\nu \psi_{\rm D}, \tag{3.74}$$

where $\psi_{\rm D}$ is the regular component of ψ in the sense of the decomposition (3.125). Here $\Lambda = (I - \Delta_{\partial\Omega})^{\frac{1}{2}}$, where $\Delta_{\partial\Omega}$ is the Laplace-Beltrami operator on $\partial\Omega$ [BGM71], and its role is merely to pull back $\partial_\nu\psi_{\rm D} \in H^{\frac{1}{2}}(\partial\Omega)$ to $\mathscr{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$, the common Hilbert space of the boundary data. Any unitary map from $H^{\frac{1}{2}}(\partial\Omega)$ to $H^{-\frac{1}{2}}(\partial\Omega)$ will do, and the reader can safely ignore its presence henceforth. For further mathematical details see [FGL17b] and Chapter 5.

3.7.1 Parametrization of the self-adjoint extensions of H by means of spectral projections

It is of interest to recast the former parametrization of H_U isolating the contribution of the eigenvalue 1 from the spectrum of U and to express it in terms of spectral projections.
In the same spirit of section 3.4 we define P_U as the eigenprojection of U with eigenvalue 1 and $Q_U = I - P_U$ its orthogonal projection.
Then, the unitary operator U can be decomposed in the sum $U = P_U + V_U$, where $V_U = Q_U\, U\, Q_U$. After projecting on the two mutually orthogonal subspaces provided by P_U and Q_U, the domain of H_U reads:

$$D(H_U) = \{\psi \in D(H^*) :\, P_U\varphi = 0\,,\, Q_U\dot\varphi = -K_U\varphi\}\,, \tag{3.75}$$

where K_U is the Cayley transform of V_U:

$$K_U = -\mathscr{C}^{-1}(V_U)Q_U = -\mathrm{i}\,(I + V_U)(I - V_U)^{-1}Q_U. \tag{3.76}$$

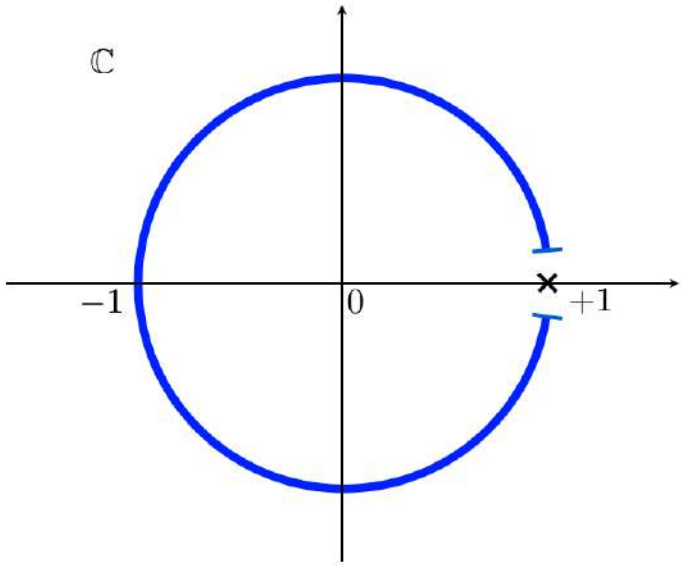

Figure 3.2: The spectrum of V_U has a gap around the point 1 in the complex plane.

Even in this higher dimensional case the operator $(I - V_U)$ is invertible, but it may be unbounded. The operator $(I - V_U)^{-1}$ will be bounded as long as the spectrum has a gap around the point 1 (Figure 3.2). For this reason, from now on, we are going to make the latter our working assumption, [ILP15b].

3.7.2 Quadratic forms

As already sketched for the one-dimensional case we provide an explicit expression for the expectation value of the kinetic energy of a free particle in a cavity Ω.

We are going to prove that the expectation value of the kinetic energy H_U is:

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_U\varphi\rangle_{\mathscr{H}_b}\right), \tag{3.77}$$

where ψ_{D} is the regular component of ψ in the sense of the decomposition (3.125), K_U is the operator defined in (3.76) and $\mathscr{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$.

Take $\psi \in D(H_U) \cap C^\infty(\overline{\Omega})$, since $D(H_U) \subset D(H^*) = D(H_{\mathrm{D}}) + N(H^*)$, it follows that every $\psi \in D(H_U)$ can be decomposed into the sum of ψ_{D} and

ψ_0. Consider:

$$\begin{aligned}\frac{2m}{\hbar^2}\, t_U(\psi) &= \langle\psi\,|-\Delta\psi\rangle_{L^2(\Omega)} = \langle\psi\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} + \langle\psi\,|-\Delta\psi_0\rangle_{L^2(\Omega)} \quad (3.78)\\ &= \langle\psi\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} = \langle\psi_{\rm D}\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} + \langle\psi_0\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)}\end{aligned}$$

where we used twice the decomposition of ψ and once the condition $-\Delta\psi_0 = 0$. Next by means of the Gauss-Green formulas (with the convention of outward ν) we will show that:

a) $\langle\psi_{\rm D}\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} = \|\nabla\psi_{\rm D}\|^2_{L^2(\Omega)}$;

b) $\langle\psi_0\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} = -\langle\psi|\partial_\nu\psi_{\rm D}\rangle_{L^2(\partial\Omega)}$;

so that, putting them both together, we obtain:

$$\frac{2m}{\hbar^2}\, t_U(\psi) = \|\nabla\psi_{\rm D}\|^2_{L^2(\Omega)} - \langle\psi|\partial_\nu\psi_{\rm D}\rangle_{L^2(\partial\Omega)}. \quad (3.79)$$

Let us begin from a):

$$\begin{aligned}\langle\psi_{\rm D}\,|-\Delta\psi_{\rm D}\rangle_{L^2(\Omega)} &= -\int_\Omega \overline{\psi_{\rm D}(x)}\,\Delta\psi_{\rm D}(x)\,{\rm d}x \quad (3.80)\\ &= \int_\Omega |\nabla\psi_{\rm D}(x)|^2\,{\rm d}x - \int_{\partial\Omega}\overline{\psi_{\rm D}}\,\partial_\nu\psi_{\rm D}\,{\rm d}S \quad (3.81)\\ &= \int_\Omega |\nabla\psi_{\rm D}(x)|^2\,{\rm d}x = \|\nabla\psi_{\rm D}\|^2_{L^2(\Omega)} \quad (3.82)\end{aligned}$$

where we used the condition that $\psi_{\rm D}|_{\partial\Omega} = 0$.
Next we move on to the computation of b). Preliminarily we prove that:

$$\langle\nabla\psi_{\rm D}|\nabla\psi_0\rangle_{L^2(\Omega)} = 0. \quad (3.83)$$

Indeed:

$$\begin{aligned}\langle\nabla\psi_{\rm D}|\nabla\psi_0\rangle_{L^2(\Omega)} &= \int_\Omega \overline{\nabla\psi_{\rm D}(x)}\cdot\nabla\psi_0(x)\,{\rm d}x \quad (3.84)\\ &= -\int_\Omega \overline{\psi_{\rm D}(x)}\,\Delta\psi_0(x)\,{\rm d}x + \int_{\partial\Omega}\overline{\psi_{\rm D}}\,\partial_\nu\psi_0\,{\rm d}S \quad (3.85)\\ &= 0 \quad (3.86)\end{aligned}$$

since $\psi_{\mathrm{D}}|_{\partial\Omega} = 0$ and $-\Delta\psi_0 = 0$. Eventually we compute b):

$$\begin{aligned}
\langle\psi_0 \,|\, -\Delta\psi_{\mathrm{D}}\rangle_{L^2(\Omega)} &= -\int_\Omega \overline{\psi_0(x)}\,\Delta\psi_{\mathrm{D}}(x)\,\mathrm{d}x && (3.87)\\
&= \int_\Omega \overline{\nabla\psi_0(x)}\cdot\nabla\psi_{\mathrm{D}}(x)\,\mathrm{d}x - \int_{\partial\Omega}\overline{\psi_0}\,\partial_\nu\psi_{\mathrm{D}}\,\mathrm{d}S && (3.88)\\
&= -\int_{\partial\Omega}\overline{\psi}\,\partial_\nu\psi_{\mathrm{D}}\,\mathrm{d}S = -\langle\psi\,|\partial_\nu\psi_{\mathrm{D}}\rangle_{L^2(\partial\Omega)} && (3.89)
\end{aligned}$$

where we made use of equation (3.83), and that $\psi_0|_{\partial\Omega} = \psi|_{\partial\Omega}$.
Putting together all the ingredients we find that for all $\psi \in D(H_U)\cap C^\infty(\overline{\Omega})$:

$$\begin{aligned}
\frac{2m}{\hbar^2}\,t_U(\psi) &= \langle\psi\,|\,-\Delta\psi\rangle_{L^2(\Omega)} && (3.90)\\
&= \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\psi|\partial_\nu\psi_{\mathrm{D}}\rangle_{L^2(\partial\Omega)} && (3.91)\\
&= \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle\psi|\Lambda\left(\partial_\nu\psi_{\mathrm{D}}\right)\rangle_{H^{-1/2}(\partial\Omega)} && (3.92)\\
&= \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle\varphi|\dot\varphi\rangle_{\mathscr{H}_b} && (3.93)\\
&= \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_U\varphi\rangle_{\mathscr{H}_b}. && (3.94)
\end{aligned}$$

where we used the definition of the inner product of $H^{-\frac{1}{2}}(\partial\Omega)$, (compare with equation (3.124) in the Appendix) and the definition of the boundary values $(\varphi,\dot\varphi)$ in (3.74). Eventually from equation (3.93) to (3.94) we used the boundary conditions in (3.75). By a density argument it follows that

$$\frac{2m}{\hbar^2}\,t_U(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_U\varphi\rangle_{\mathscr{H}_b}, \qquad \text{for all } \psi\in D(H_U). \tag{3.95}$$

The mathematical expression of t_U for the kinetic energy of a free particle in a cavity Ω highly resembles the one determined in equation (3.29) for the one-dimensional case. Though this apparent similarity, the two equations differ considerably. For example the contribution from the bulk is due to the regular part of ψ, that is ψ_{D}, rather than from the whole function. Moreover, the border contribution is bounded as long as K_U is bounded, which is guaranteed by the condition of gapped spectrum for V_U.

Eventually, since $D(H_U)$ is a core for $D(t_U)$ we find that:

$$D(t_U) = \{\psi \in H_0^1(\Omega) + N(H^*) \,:\, P_U\varphi = 0\}, \tag{3.96}$$

where $H_0^1(\Omega)$ is the subspace of $H^1(\Omega)$ whose elements vanish at the boundary. For more details see [FGL17b].

3.7.3 Composition law in a cavity

We now evaluate the limit of the alternating dynamics (3.10) in the case of a free particle confined in a cavity $\Omega \subset \mathbb{R}^n$. Once more the product formula (3.10) holds with the form sum

$$H_W = \frac{H_{U_1} \dot{+} H_{U_2}}{2}. \tag{3.97}$$

Following the one-dimensional case we carry on the computation of the sum:

$$\begin{aligned} t_{12}(\psi) &= \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{\hbar^2}{2m}\left(\|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_{12}\varphi\rangle_{\mathscr{H}_b}\right), \\ K_{12} &= \frac{1}{2}\left(K_{U_1} + K_{U_2}\right), \end{aligned} \tag{3.98}$$

and its domain

$$D(t_{12}) = \{\psi \in H_0^1(\Omega) + N(H^*) \,:\, P_{12}\varphi = 0\}. \tag{3.99}$$

We stress that K_{12} is a bounded self-adjoint operator, since both K_{U_1} and K_{U_2} are, thus the quadratic form t_{12} is closed and bounded from below. Therefore, by the representation theorem [Kat66], there exists a unique self-adjoint extension H_W of H such that

$$t_{12}(\psi) = \langle\psi|H_W\psi\rangle_{L^(\Omega)}, \qquad \text{for all } \psi \in D(H_W), \tag{3.100}$$

where

$$D(H_W) = \{\psi \in D(H^*) \,:\, \mathrm{i}(I+W)\varphi = (I-W)\dot{\varphi}\}. \tag{3.101}$$

We stress that $P_W = P_{12}$, so that W can be explicitly built from $\{P_{12}, Q_{12}\}$:

$$W = P_{12} - \mathscr{C}(K_{12})Q_{12} \tag{3.102}$$

where $\mathscr{C}(K_{12})$ is the Cayley transform of K_{12} on the range of Q_{12}. This complete our proof of Eq. (3.12).

3.8 Example

We would like to provide the reader with an example of composition law in the n dimensional case. Let us consider the following unitary operator on $L^2(\partial\Omega)$

$$(U\Phi)(x) = \mathrm{e}^{i\alpha(x)}\Phi(x) \quad , \quad x \in \partial\Omega \tag{3.103}$$

where α is a function such that $0 \leq \alpha(x) < 2\pi$ and $\left(1 - \mathrm{e}^{i\alpha(\cdot)}\right)^{-1}$ is essentially bounded. The former operator can be extended to a unitary operator on $\mathscr{H}_b$ making use of the operator $\Lambda_{1/2} \equiv \sqrt{\Lambda}$, namely:

$$\Lambda_{1/2} : L^2(\partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega) \tag{3.104}$$

$$\Lambda_{1/2} = (I - \Delta_{\partial\Omega})^{\frac{1}{4}}, \tag{3.105}$$

so that the operator $\Lambda_{1/2} U \Lambda_{1/2}^{\dagger}$ is a unitary operator on $\mathscr{H}_b$. For the sake of simplicity we will keep on using the same letter U to indicate the unitary operator on $\mathscr{H}_b$.

Let us compare equation (3.103) with equation (3.24). In the one dimensional case, where the boundary was made only by two points, the unitary matrix U in equation (3.24) was completely determined by two complex numbers, α_1 and α_2.

In other words, we were able to effectively describe the physics at the boundary of the interval by means of α_1 and α_2. In the case of a cavity Ω in $\mathbb{R}^n$, we need to assign a value of α for every point in $\partial\Omega$. In this manner, equation (3.103) reads like a generalization of Robin boundary conditions in equation (3.24).

Let us move on to the decomposition of U in terms of P_U and Q_U:

$$P_U = \chi_{\{1\}}(U) = \chi_{\alpha^{-1}(\{0\})}, \tag{3.106}$$

$$Q_U = 1 - \chi_{\{1\}}(U) = \chi_{\alpha^{-1}(\mathbb{R}\setminus\{0\})}, \tag{3.107}$$

so that, the operator U restricted to the range of Q_U reads:

$$V_U = Q_U U Q_U = \mathrm{e}^{i\alpha(x)}\chi_{\alpha^{-1}(\mathbb{R}\setminus\{0\})}. \tag{3.108}$$

The last fundamental ingredient is provided by the Cayley transform of V_U,

$$K_U = -\mathrm{i}\,(I+V_U)(I-V_U)^{-1}Q_U = -i\,\frac{1+\mathrm{e}^{i\alpha(x)}}{1-\mathrm{e}^{i\alpha(x)}}\chi_{\alpha^{-1}(\mathbb{R}\setminus\{0\})}. \tag{3.109}$$

We recall that K_U is bounded since the function $x \mapsto \left(1-\mathrm{e}^{i\alpha(x)}\right)^{-1}$ is essentially bounded.
Let us consider the following unitary operators U_1 and U_2:

$$(U_1\Phi)(x) = \mathrm{e}^{i\alpha_1(x)}\Phi(x), \tag{3.110}$$

$$(U_2\Phi)(x) = \mathrm{e}^{i\alpha_2(x)}\Phi(x), \tag{3.111}$$

$x \in \partial\Omega$, and compute $U_1 * U_2$. Moreover, we suppose that the maps $x \mapsto (1-\mathrm{e}^{i\alpha_1(x)})^{-1}$ and $x \mapsto (1-\mathrm{e}^{i\alpha_2(x)})^{-1}$ are both essentially bounded. We are going to check that:

$$\begin{aligned} U_1 * U_2 &= P_{12} - \mathscr{C}(K_{12})Q_{12} && (3.112)\\ &= \chi_{\alpha_1^{-1}(\{0\})\cup\alpha_2^{-1}(\{0\})} - \mathrm{e}^{i(\alpha_1+\alpha_2)}\frac{\overline{z}}{z}\chi_{\alpha_1^{-1}(\mathbb{R}\setminus\{0\})\cap\alpha_2^{-1}(\mathbb{R}\setminus\{0\})}, && (3.113)\end{aligned}$$

where $z = 2 - \mathrm{e}^{i\alpha_1} - \mathrm{e}^{i\alpha_2}$.
Let us start from the projections. From the very definition of Q_{12} we know that $\mathrm{Ran}(Q_{12}) = \mathrm{Ran}(Q_{U_1}) \cap \mathrm{Ran}(Q_{U_2})$. Since:

$$\mathrm{Ran}(Q_{U_1}) = \{\chi_{\alpha_1^{-1}(\mathbb{R}\setminus\{0\})}f : f \in \mathscr{H}_b\} \tag{3.114}$$

$$\mathrm{Ran}(Q_{U_2}) = \{\chi_{\alpha_2^{-1}(\mathbb{R}\setminus\{0\})} f : f \in \mathscr{H}_b\} \tag{3.115}$$

we can infer that $\mathrm{Ran}(Q_{12}) = \mathrm{Ran}(Q_{U_1}) \cap \mathrm{Ran}(Q_{U_2}) = \{\chi_{\alpha_1^{-1}(\mathbb{R}\setminus\{0\})\cap\alpha_2^{-1}(\mathbb{R}\setminus\{0\}} f : f \in \mathscr{H}_b\}$. Thus it follows that:

$$Q_{12} = \chi_{\alpha_1^{-1}(\mathbb{R}\setminus\{0\})\cap\alpha_2^{-1}(\mathbb{R}\setminus\{0\})} \tag{3.116}$$

$$P_{12} = \chi_{\alpha_1^{-1}(\{0\})\cup\alpha_2^{-1}(\{0\})} \tag{3.117}$$

Let us move on to K_{12}:

$$K_{12} = \frac{1}{2}\left(K_{U_1} + K_{U_2}\right) = -i\,\frac{1-\mathrm{e}^{i(\alpha_1+\alpha_2)}}{\left(1-\mathrm{e}^{i\alpha_1}\right)\left(1-\mathrm{e}^{i\alpha_2}\right)} Q_{12}. \tag{3.118}$$

Eventually we compute $\mathscr{C}(K_{12})Q_{12}$. After a straightforward computation it follows that:

$$\mathscr{C}(K_{12})Q_{12} = -\frac{\mathrm{e}^{i\alpha_1} + \mathrm{e}^{i\alpha_2} - 2\mathrm{e}^{i(\alpha_1+\alpha_2)}}{2-\mathrm{e}^{i\alpha_1}-\mathrm{e}^{i\alpha_2}} Q_{12} = \mathrm{e}^{i(\alpha_1+\alpha_2)}\frac{\overline{z}}{z} Q_{12}. \tag{3.119}$$

where $z = 2 - \mathrm{e}^{i\alpha_1} - \mathrm{e}^{i\alpha_2}$. Then, plugging the previous expressions in the right places, equation (3.113) follows.
Interestingly it happens that on the points of $\partial\Omega$ where either $\alpha_1 = 0$ or $\alpha_2 = 0$, Dirichlet boundary conditions prevail, indeed:

$$P_{12} = \chi_{\alpha_1^{-1}(\{0\})\cup\alpha_2^{-1}(\{0\})} = 1. \tag{3.120}$$

Another interesting situation happens on the points where $\alpha_1 = \pi$ (Neumann boundary conditions, $U_1 = -\mathbb{I}$) and $\alpha_2 \neq 0$. In this case the projections read $P_{12} = 0$ and $Q_{12} = 1$, while $\mathscr{C}(K_{12})Q_{12} = -\mathrm{e}^{i\alpha_2}\frac{\overline{z}}{z} = U_2\frac{\overline{z}}{z}$.

3.9 Final remarks

In this section we are going to consider the generalization of the composition law to boundary unitaries U_i, which are not gapped, and thus to unbounded K_{U_i}. In general, the sum of two unbounded (self-adjoint) operators $K_{U_1}+K_{U_2}$ is a touchy business. However, if the two operators are bounded from below,

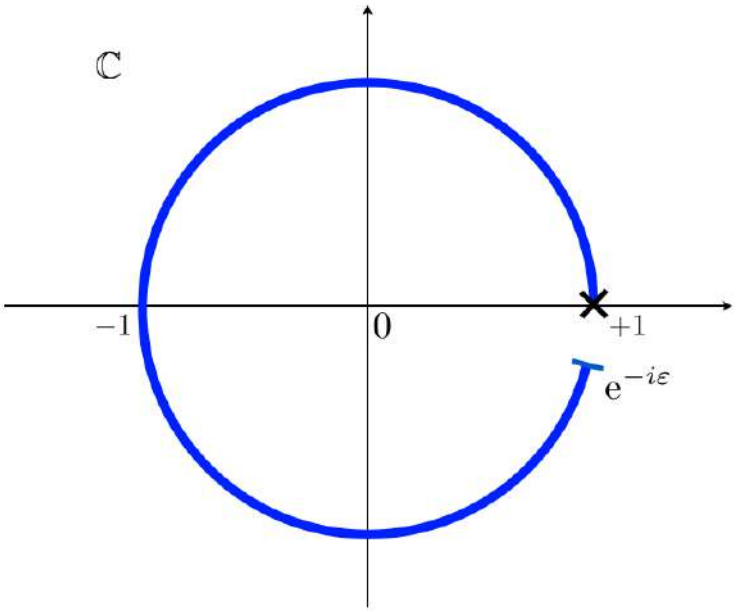

Figure 3.3: If K_U is lower bounded, say $K_U \geq \beta$, then the spectrum of V_U has a semi-gap around the point 1 in the spectrum.

the situation can be kept somewhat under control.

It can be proved [Gru74] that a self-adjoint extension of H, say H_U, is bounded from below as long as the corresponding operator H_U, which appears in equation (3.76), is bounded from below. By the properties of the Cayley transform it is easy to see that K_U is bounded from below, if and only the spectrum of U has a gap just below the point 1, namely the set $\{e^{i\alpha} : \alpha \in (-\varepsilon, 0)\}$ belongs to the resolvent set of U for some $\varepsilon > 0$. We will call such a U semi-gapped. See figure 3.3, where $\beta = -\cot(\varepsilon/2)$.

Suppose that H_{U_1} and H_{U_2} are lower-bounded self-adjoint operators. We remind the reader that the hypothesis of lower-boundedness is fundamental in order to let the Trotter-Kato formula in equation (3.7) hold. Next, consider the quadratic form:

$$t_{12}(\psi) = \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{\hbar^2}{2m}\left(\|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\varphi|K_{12}\varphi\rangle_{\mathscr{H}_b}\right),$$
$$K_{12} = \frac{1}{2}\left(K_{U_1} + K_{U_2}\right) \qquad D(K_{12}) = D(K_1) \cap D(K_2) \quad (3.121)$$

defined on

$$D(t_{12}) = D(t_{U_1}) \cap D(t_{U_2}) = \{\psi \in H_0^1(\Omega) + N(H^*) \,:\, P_{12}\varphi = 0\} \cap \gamma^{-1}(D(K_{12})), \tag{3.122}$$

where

$$\gamma^{-1}(D(K_{12})) = \{\psi \in L^2(\Omega) : \psi|_{\partial\Omega} \in D(K_{12}) \subset \mathscr{H}_b\}. \tag{3.123}$$

Now suppose that K_{12} is self-adjoint on $N(P_{12})$. It may happen, in fact, that the sum of K_1 and K_2 is not self-adjoint and the former construction would be meaningless, because $D(K_1) \cap D(K_2)$ could even reduce to the zero vector. In particular, it is sufficient, for example, that either K_1 or K_2 is bounded, so that their sum would surely be self-adjoint. The latter situation happens when, for example, $1 \in \rho(V_{U_1})$, the resolvent set of V_{U_1}, that is when U is gapped.
Then, by the representation theorem in [FGL17b] the form t_{12} is the expectation value of a self-adjoint operator, H_W (W being a unitary operator on $\mathscr{H}_b$), which is the form sum operator of H_{U_1} and H_{U_2}, namely $H_W = \frac{H_{U_1} \dot{+} H_{U_2}}{2}$. Note that, by the previous discussion it follows that H_W is lower bounded because K_{12} is.

3.10 Appendix

In this appendix we would like to give some more details about the role of boundary data in equation (3.74).
We recall that, for any $s \in \mathbb{R}$, $H^s(\partial\Omega)$ is a Hilbert space whose inner product is defined as:

$$\langle \phi_1 | \phi_2 \rangle_{H^s(\partial\Omega)} = \langle \Lambda^s \phi_1 | \Lambda^s \phi_2 \rangle_{L^2(\partial\Omega)} = \int_{\partial\Omega} \overline{\Lambda^s \phi_1(x)} \Lambda^s \phi_2(x) \, \mathrm{d}S \tag{3.124}$$

where $\phi_1, \phi_2 \in H^s(\partial\Omega)$, $\Lambda = (I - \Delta_{\partial\Omega})^{\frac{1}{2}}$ and $\Delta_{\partial\Omega}$ is the Laplace-Beltrami operator on $\partial\Omega$ [BGM71]. Moreover it will be crucial in what follows that Λ is a unitary operator from $H^{\frac{1}{2}}(\partial\Omega)$ to $H^{-\frac{1}{2}}(\partial\Omega)$ [Fol99]. As a remark, the

regularity of the functions in $H^s(\partial\Omega)$ increases with s: if $s = 0$, $H^0(\partial\Omega) = L^2(\partial\Omega)$, if $s > 0$ then $H^s(\partial\Omega)$ contains functions with "derivatives of order s", while $H^{-s}(\partial\Omega)$ is the space of distributions obtained as the dual of $H^s(\partial\Omega)$. For this reason equation (3.19) cannot hold by naively interpreting the boundary data $(\varphi, \dot{\varphi})$ as the couple $(\psi|_{\partial\Omega}, \partial_\nu\psi)$. Indeed, the elements in the couple are settled on different Hilbert spaces ($H^{-\frac{1}{2}}(\partial\Omega)$ and $H^{-\frac{3}{2}}(\partial\Omega)$) and the existence of an operator U acting both on $\psi|_{\partial\Omega}$ and $\partial_\nu\psi$ becomes meaningless. As we are going to discuss, only the most regular component of the normal derivative will contribute to the boundary data.
In order to define the regular component ψ_{D} of ψ, we need a useful decomposition of $D(H^*)$:

$$D(H^*) = D(H_{\mathrm{D}}) + N(H^*), \tag{3.125}$$

where H_{D} is the self-adjoint extension of H with Dirichlet boundary conditions, that is $H_{\mathrm{D}}\psi = -\frac{\hbar^2}{2m}\Delta\psi$ on the domain

$$D(H_{\mathrm{D}}) = \{\psi \in H^2(\Omega) : \psi|_{\partial\Omega} = 0\}, \tag{3.126}$$

and

$$N(H^*) = \{\psi \in D(H^*) : -\Delta\psi = 0\}. \tag{3.127}$$

In this appendix we provide the reader with some further details about the above decomposition of $D(H^*)$, which is is crucial to define the regularized normal derivative of a wave function and its boundary data $(\varphi, \dot{\varphi})$ in (3.74). Using this decomposition, every $\psi \in D(H^*)$ can be uniquely decomposed in the sum $\psi_{\mathrm{D}} + \psi_0$, where $\psi_{\mathrm{D}} \in D(H_{\mathrm{D}})$ is a function vanishing on the border, $\psi_{\mathrm{D}}|_{\partial\Omega} = 0$, and ψ_0 is a harmonic function, $-\Delta\psi_0 = 0$. Thus the boundary data are defined as in equation (3.74):

$$\begin{cases} \varphi = \psi|_{\partial\Omega}, \\ \dot{\varphi} = \Lambda\left(\partial_\nu\psi_{\mathrm{D}}\right). \end{cases} \tag{3.128}$$

so that both the elements at the border are settled on the same Hilbert space $\mathscr{H}_b$.

Let's get an inner view on the decomposition $D(H^*) = D(H_{\rm D}) + N(H^*)$, which turned out to be very useful to define the regularized normal derivative of a wave function and the boundary values $(\varphi, \dot{\varphi})$.
In order to understand the meaning of this decomposition, we explain here how to decompose a smooth wave function $\psi \in C^\infty(\overline{\Omega}) \subset D(H^*)$ into the sum $\psi = \psi_{\rm D} + \psi_0$, with $\psi_{\rm D}|_{\partial\Omega} = 0$ and $-\Delta\psi_0 = 0$. First of all we define g as $\psi|_{\partial\Omega}$ and solve the (boundary value) electrostatic problem:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ u = g & \text{on } \partial\Omega \end{cases}. \tag{3.129}$$

The solution ψ_0 of (3.129) represents the electrostatic potential in the cavity Ω with the given value $g = \psi|_{\partial\Omega}$ on the boundary. In other words ψ_0 is a harmonic function such that its value along the border is exactly $g = \psi|_{\partial\Omega}$. Next, we define $\psi_{\rm D}$ as $\psi - \psi_0$; manifestly $\psi_{\rm D}|_{\partial\Omega} = 0$. Therefore we can write $\psi = \psi_{\rm D} + \psi_0$ with $\psi_{\rm D}|_{\partial\Omega} = 0$ and $-\Delta\psi_0 = 0$. As a technical remark this decomposition can be extended by density arguments up to $D(H^*)$ (see [Gru09]), that is: $D(H^*) = D(H_{\rm D}) + N(H^*)$ where:

$$D(H_{\rm D}) = \{\psi \in H^2(\Omega) : \psi|_{\partial\Omega} = 0\} \tag{3.130}$$

$$N(H^*) = \{\psi \in D(H^*) \, : \, -\Delta\psi = 0\}, \tag{3.131}$$

Notice that $D(H_{\rm D})$ represents the domain of a self-adjoint extension of H (the one specified by Dirichlet boundary conditions) and it is made up by much more regular functions than $N(H^*)$.
Indeed, the space $N(H^*)$ contains functions that can be very irregular on $\partial\Omega$. This is a fairly interesting phenomenon in potential theory: a harmonic functions, which is extremely regular (analytic) in the interior of Ω can become very irregular on its boundary.
For example, consider $\Omega = \mathbb{R}^2_+ = \{(x, y) \in \mathbb{R}^2 : y > 0\}$ and define the function $f : \Omega \to \mathbb{C}$, $f(x, y) = (x + \mathrm{i}y)^{-1}$. It is well known that though being harmonic on $\Omega = \mathbb{R}^2_+$, the function f is ill-defined on $\partial\Omega$. Indeed, from the

theory of distributions:

$$\lim_{y\downarrow 0} f(z) = P.V.\frac{1}{x} - \mathrm{i}\pi\delta(x), \tag{3.132}$$

where *P.V.* denotes the Cauchy principal value and δ the Dirac delta. Moreover $N(H^*)$ is also responsible for the lack of self-adjointness of T as outlined in the theory of self-adjoint extensions designed by von Neumann [Neu55].

Chapter 4

Boundaries without boundaries

In this chapter we are going to answer to the following question: *Can one generate boundary conditions starting from a quantum system on a manifold without boundaries?* [Fac+17]
Starting with a closed manifold without boundary, we consider the process of *generating* boundaries by modding out by a group action with fixed points. As an illustrative example, we consider the special case of $\mathbb{S}$ and generate the interval $[0, \pi]$ via parity reduction. We, eventually, study the generation of boundary conditions by means of a folding procedure, with the introduction of an auxiliary ancilla space.

4.1 Generation of boundary conditions by reduction

In this section we show a way of generating boundary conditions for a non-relativistic particle on a manifold without boundaries. We first recall how to obtain a manifold with boundaries as a quotient of the action of a group of transformations on a manifold without boundaries. In particular we will focus on the unit circle and the action of $\mathbb{Z}_2$ on it, which makes the unit circle collapse into an interval.

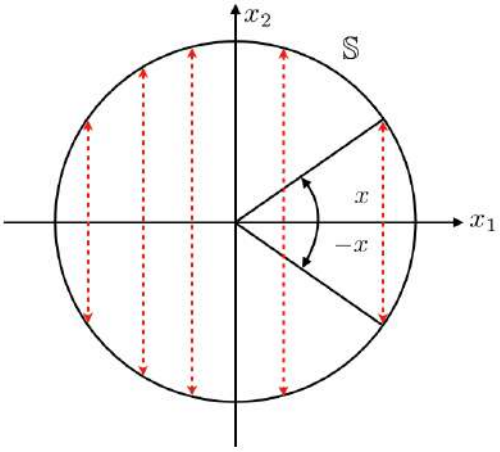

Figure 4.1: Identification of symmetric points of the unit circle $\mathbb{S}$ by means of Π.

We will now consider a free quantum particle on the unit circle, a compact manifold without boundary, and will implement a procedure to generate boundary conditions on the quotient manifold with boundaries.
The unit circle in the plane $\mathbb{R}^2$ is defined by

$$\mathbb{S} = \{(x_1, x_2) \in \mathbb{R}^2 \,|\, x_1^2 + x_2^2 = 1\}, \tag{4.1}$$

and can be parametrized, in $\mathbb{S} \setminus \{(-1, 0)\}$, by

$$x \in (-\pi, \pi) \to \begin{cases} x_1 = \cos x, \\ x_2 = \sin x. \end{cases} \tag{4.2}$$

It is possible to generate an interval of the real line by modding out the unit circle by a parity transformation. Consider the map

$$\Pi : \mathbb{S} \to \mathbb{S}, \qquad \Pi(x_1, x_2) = (x_1, -x_2), \tag{4.3}$$

or in terms of $x \in (-\pi, \pi)$, $\Pi(x) = -x$. Manifestly, Π is a bijection and an involution, since $\Pi^2 = \mathbb{I}$.
The action of Π on the unit circe $\mathbb{S}$ (see Figure 4.1) identifies pairs of points on the circle and admits only two fixed points, namely $(1, 0)$ and $(-1, 0)$.

With the aid of the transformation Π we are identifying symmetric points, or, equivalently, puncturing the circle in $(1,0)$ and $(-1,0)$, and pushing the lower semicircle onto the upper one.
This is mathematically achieved by considering the quotient space of the unit circle under the action of the discrete group $\mathbb{Z}_2$. Indeed, the space of (discrete) orbits determined by Π,

$$M = \mathbb{S}/\Pi, \tag{4.4}$$

is the interval $\mathbb{S}_+ = [0, \pi]$ (or, equivalently, the interval $\mathbb{S}_- = [-\pi, 0]$). Thus, by taking the quotient of the unit circle by the discrete action of Π we obtain a one dimensional manifold with boundary $M = \mathbb{S}_+$.
Now we will represent the action of Π on square integrable functions on $\mathbb{S}$, and show how boundary conditions are going to emerge after this process.
The action of Π on functions can be implemented by a pull-back

$$P : L^2(\mathbb{S}) \to L^2(\mathbb{S}), \qquad (P\psi)(x) = \psi(\Pi(x)) = \psi(-x). \tag{4.5}$$

Moreover $P^2 = \mathbb{I}$, so that the eigenspaces of the parity operator P belong to the eigenvalues ± 1.
The action of P splits the Hilbert space $L^2(\mathbb{S})$ into two mutually orthogonal subspaces $\mathcal{H}_+$ and $\mathcal{H}_-$, defined by

$$\mathcal{H}_\pm = \{\psi \in L^2(\mathbb{S}) \,|\, P\psi = \pm\psi\}. \tag{4.6}$$

Notice that $L^2(\mathbb{S})$ can be identified with $L^2(-\pi, \pi)$, the Hilbert space of square integrable functions on the interval $(-\pi, \pi)$. Under such identification we get

$$\mathcal{H}_\pm = \{\psi \in L^2(-\pi, \pi) \,|\, \psi(-x) = \pm\psi(x)\}, \tag{4.7}$$

that is the set of even and odd functions on $(-\pi, \pi)$, respectively.
Consider the Hamiltonian of a free particle on a circle (1.19). Since $\mathbb{S}$ is a compact manifold without boundary, the Laplace operator is essentially self-adjoint on $C^\infty(\mathbb{S}) = C_c^\infty(\mathbb{S})$, the smooth function on the circle [Jos11].

The domain of self-adjointness is the second Sobolev space $H^2(\mathbb{S})$, which, in coordinates reads

$$H^2(\mathbb{S}) = \{\psi \in H^2[-\pi,\pi] : \psi(-\pi) = \psi(\pi)\,,\, \psi'(-\pi) = \psi'(\pi)\}. \tag{4.8}$$

Here, $H^2[-\pi,\pi]$ is the set of square-integrable functions, with square-integrable (first and) second distribution derivative.
Interestingly the parity operator P and the operator H commutes on $H^2(\mathbb{S})$:

$$H\,P = P\,H. \tag{4.9}$$

This is a crucial ingredient in our construction, which we remind consists in obtaining a self-adjoint operator on the quotient space, say the interval $[0,\pi]$, starting from the operator H on the unit circle.
From the commutation relation $HP = PH$ it follows that whenever the operator H acts on $\mathcal{H}_+$ (respectively on $\mathcal{H}_-$) then its image remains in $\mathcal{H}_+$ (respectively in $\mathcal{H}_-$). Thus, the restriction of H to one of the two subspaces gives rise to a self-adjoint operator. We are going to show that the restrictions of H to these parity eigenspaces can be identified with two self-adjoint Hamiltonian operators on the interval $[0,\pi]$.
From (4.7) and (4.8), one has

$$D(H|_{\mathcal{H}_+}) = H^2(\mathbb{S}) \cap \mathcal{H}_+ = \{\psi \in H^2[-\pi,\pi] \cap \mathcal{H}_+ : \psi'(-\pi) = 0 = \psi'(\pi)\}. \tag{4.10}$$

Since the space of square integrable even functions ψ on the interval $(-\pi,\pi)$ is unitarily equivalent to the space of square integrable functions ϕ on $(0,\pi)$, the domain in equation (4.10) can be recast on the interval $\mathbb{S}_+ = [0,\pi]$. Indeed, define the following unitary operator

$$\begin{aligned} &U_+ : \mathcal{H}_+ \to L^2(0,\pi), \qquad \phi(x) = (U_+\psi)(x) = \sqrt{2}\,\psi(x), \quad x \in \mathbb{S}_+, \\ &U_+^\dagger : L^2(0,\pi) \to \mathcal{H}_+, \qquad \psi(x) = (U_+^\dagger\phi)(x) = \frac{1}{\sqrt{2}} \begin{cases} \phi(x), & x \in \mathbb{S}_+, \\ \phi(-x), & x \in \mathbb{S}_-. \end{cases} \end{aligned} \tag{4.11}$$

Then we have

$$H_+ := U_+ \, H|_{\mathcal{H}_+} \, U_+^\dagger = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{4.12}$$

$$D(H_+) = \{\psi \in H^2[0,\pi] : \psi'(0) = 0 = \psi'(\pi)\}, \tag{4.13}$$

where the derivative at 0 must vanish, because even functions have odd derivatives. Equation (4.13) can be immediately read on the quotient space $\mathbb{S}_+ = [0,\pi]$, as a self-adjoint extension of the Hamiltonian describing a free particle on the interval $[0,\pi]$ with *Neumann* boundary conditions.
Similarly, for the subspace of odd functions $\mathcal{H}_-$, we get

$$D(H|_{\mathcal{H}_-}) = H^2(\mathbb{S}) \cap \mathcal{H}_- = \{\psi \in H^2[-\pi,\pi] \cap \mathcal{H}_- : \psi(-\pi) = 0 = \psi(\pi)\}, \tag{4.14}$$

and we can define the unitary operator between the space of square integrable odd functions ψ on $(-\pi,\pi)$ and the space of square integrable functions ϕ on $(0,\pi)$ acting as

$$\begin{aligned} &U_- : \mathcal{H}_- \to L^2(0,\pi), \qquad \phi(x) = (U_-\psi)(x) = \sqrt{2}\,\psi(x), \quad x \in \mathbb{S}_+, \\ &U_-^\dagger : L^2(0,\pi) \to \mathcal{H}_-, \qquad \psi(x) = (U_-^\dagger\phi)(x) = \frac{1}{\sqrt{2}} \begin{cases} \phi(x), & x \in \mathbb{S}_+, \\ -\phi(-x), & x \in \mathbb{S}_-. \end{cases} \end{aligned} \tag{4.15}$$

Then, the restricted operator can be unitarily mapped into

$$H_- = U_- \, H|_{\mathcal{H}_-} \, U_-^\dagger = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{4.16}$$

$$D(H_-) = \{\psi \in H^2[0,\pi] : \psi(0) = 0 = \psi(\pi)\}. \tag{4.17}$$

In this case we have obtained a free particle on an interval with *Dirichlet* boundary conditions.
Summing up, we started from a self-adjoint operator H on the unit circle $\mathbb{S}$, which generates a unitary dynamics for the free particle on the circle. Besides, we picked out the eigenspaces of the parity P, say $\mathcal{H}_+$ and $\mathcal{H}_-$, which are left invariant by the one-parameter unitary group generated by H, since

$[H, P] = 0$. Therefore, the operator H restricted to the invariant subspaces $\mathcal{H}_{\pm}$, is still self-adjoint. Finally, the operators restricted to $\mathcal{H}_{+}$ and $\mathcal{H}_{-}$ can be read as two different self-adjoint realizations of the one-dimensional free Hamiltonian (1.19) on the interval $[0, \pi]$, with different boundary conditions.

4.2 The general framework

In the previous section we have shown how to generate boundary conditions on an interval starting from a unitary dynamics on the circle. In this section we would like to provide the reader with the general construction.
Consider a finite dimensional complex vector bundle $E \to M$ on a manifold M carrying a Hermitian product. In the following we are going to denote the typical fiber by V and the space of square integrable sections of E by $L^2(M, V)$. Moreover, we suppose that the bundle is parallelizable. Consider a set of fiberwise maximal pairwise commuting operators acting as a discrete group G on M.
We denote by $\tilde{M} = M/G$ the orbifold obtained in the quotient process which can happen to be a manifold with boundary or with corners. The maximality of the set implies that E admits a vector field of eigenvectors of this maximal set of operators. We obtain several copies of $L^2(\tilde{M}, \mathbb{C})$, when we consider the Hilbert space of square integrable sections with values in a given joint eigenspace.
Next, consider a one-parameter group of unitary bundle automorphisms on E, say $U(t) : E \to E$, such that $G\,U(t) = U(t)\,G$. The latter condition implies that the one-parameter unitary group leaves unchanged every single copy of $L^2(\tilde{M}, \mathbb{C})$ and its infinitesimal generator still remains self-adjoint on the Hilbert space $L^2(\tilde{M}, \mathbb{C})$ associated to a given eigenvector. In general, with each eigenvector (one dimensional eigenspace), we obtain a different self-adjoint generator.

4.2.1 Example 1

Let M be a compact Riemannian manifold without boundary. The Laplace-Beltrami operator is essentially self-adjoint, therefore its closure will generate a one-parameter group of unitary transformations on any complex vector bundle on M, with infinitesimal action $\Delta \otimes \mathbb{I}_n$ on the sections, where $\mathbb{I}_n$ is the identity matrix on $\mathbb{C}^n$. We can consider a discrete group acting on E in terms of unitary transformations and extract from it a maximal set of fiberwise commuting operators.

In this manner we get a decomposition of the fiber V into one-dimensional vector spaces and therefore $L^2(M, V)$ will be a direct sum of complex-valued square integrable functions. We select a basis of the complex-vector bundle, which is assumed to be parallelizable. With a unitary transformation it is always possible to consider a basis of eigenvectors of the commuting elements of the discrete group G.

If the action commutes with $\Delta \otimes \mathbb{I}_n$ we return to the general arguments. As our operator is $\Delta \otimes \mathbb{I}_n$ it is clear that we only need our operator to commute with the action of the discrete group on M so that it will be projectable onto $\tilde{M}$.

We should notice that, while Δ will be in the enveloping algebra of first order differential operators acting on M, say vector fields acting on M, the same property will not hold true on $\tilde{M}$, because the projected Laplacian $\tilde{\Delta}$, does not need to be in the enveloping algebra of the derivations of $\mathcal{F}(\tilde{M})$.

For example let $M = \mathbb{S}^2 = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \,|\, x_1^2 + x_2^2 + x_3^2 = 1\}$ and consider $\Delta = J_x^2 + J_y^2 + J_z^2$ and $\Pi : (x_1, x_2, x_3) \in \mathbb{R}^3 \to (x_1, x_2, -x_3)$. The quotient space will be a disk, a manifold with a smooth boundary. The operator J_z will pass to the quotient but J_x and J_y will not.

As a second example, consider again the free particle on a circle. Then $M = \mathbb{S}$, the Laplace operator $\Delta = \partial_{x_1}^2 + \partial_{x_2}^2$ and the parity transformation $\Pi : (x_1, x_2) \to (x_1, -x_2)$. Let us denote by x a coordinate of M/Π, and with $\tilde{\Delta}$ the Laplace operator on M/Π, say $\tilde{\Delta} = \partial_x^2$. The only complete vector field will be $(x-1)(x+1)\partial_x$, therefore we have to investigate the domains of self-adjointness without being able to rely on the Lie algebra of complete

vector fields acting on the quotient.

4.2.2 Example 2

Let us consider the case of a spin-1/2 particle on the unit circle. In this case we have to consider the bundle $\mathbb{S} \times \mathbb{C}^2 \to \mathbb{S}$, and apply the former construction to sections of $L^2(\mathbb{S}, \mathbb{C}^2)$.
We consider the operator $P : \psi(x_1, x_2) \to (n \cdot \sigma)\psi(x_1, -x_2)$, where n is a unit vector in $\mathbb{R}^3$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, the vector of the three Pauli matrices. For the sake of simplicity we can consider the unit vector $n = (0, 0, 1)$, so that the operator P reads $P\psi(x_1, x_2) = \sigma_3\psi(x_1, -x_2)$.
Since $P^2 = I$, the operator P admits only two eigenvalues, say ± 1, which split the Hilbert space $L^2(\mathbb{S}, \mathbb{C}^2)$ into $\mathcal{K}_+ \oplus \mathcal{K}_-$, where $\mathcal{K}_\pm$ are the eigenspaces of P with eigenvalues ± 1. More explicitly:

$$\mathcal{K}_+ = \left\{ \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in L^2(\mathbb{S}, \mathbb{C}^2) : \psi_1 \in \mathcal{H}_+, \psi_2 \in \mathcal{H}_- \right\}, \tag{4.18}$$

$$\mathcal{K}_- = \left\{ \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \in L^2(\mathbb{S}, \mathbb{C}^2) : \psi_1 \in \mathcal{H}_-, \psi_2 \in \mathcal{H}_+ \right\}, \tag{4.19}$$

where $\mathcal{H}_+$ and $\mathcal{H}_-$ are, respectively, the space of even and odd functions on the circle as given in equation (4.7). Thus $\mathcal{K}_+ = \mathcal{H}_+ \oplus \mathcal{H}_-$ and since the Laplace operator, $\Delta \otimes \mathbb{I}$, commutes with the operator P, the dynamics can be projected on $\tilde{M}$, the segment, and once again we can find Dirichlet or Neumann boundary conditions. In the same manner we obtain the same boundary conditions working with $\mathcal{K}_-$
To get additional extensions we might consider the fiber bundle $\mathbb{S} \times \mathbb{C}^4 \to \mathbb{S}$, where the parity transformations may be implemented by $\{\sigma_3 \otimes \sigma_3, \sigma_0 \otimes \sigma_0, \sigma_0 \otimes \sigma_3, \sigma_3 \otimes \sigma_0\}$. We could use $G = \{\sigma_3 \otimes \sigma_0, \sigma_0 \otimes \mathfrak{u}(2)\}$ with maximal pairwise commuting operators $\{\sigma_3 \otimes \sigma_0, \sigma_0 \otimes n \cdot \sigma, \sigma_0 \otimes \sigma_0, \sigma_3 \otimes n \cdot \sigma\}$. In this manner we should obtain additional self-adjoint extensions of the Laplace operator on the interval.

4.3 General boundary conditions

In section 4.1 we showed how to obtain Dirichlet and Neumann boundary conditions by a reduction of the free dynamics on the circle. Now we would like to get general boundary conditions. We can move from functions on $\mathbb{S}$ to sections and consider covariant derivatives instead of ordinary ones. Any section over the circle can be trivialized at the cost of bringing in a connection and replacing ordinary derivatives with covariant ones.
We are thus considering a U(1) principal fiber bundle. We write:

$$A = i\alpha(x)\mathrm{d}x, \tag{4.20}$$

$$D\psi = \mathrm{d}\psi + A\psi, \tag{4.21}$$

where d is the exterior derivative. We must ensure that the connections are projectable under the map P:

$$P\,D = D\,P. \tag{4.22}$$

Applying this expression on a section we get

$$\mathrm{d}\psi(-x) + A(-x)\psi(-x) = \mathrm{d}\psi(-x) + A(x)\psi(-x), \tag{4.23}$$

which implies that

$$\alpha(x) = -\alpha(-x), \tag{4.24}$$

and $\alpha(0) = 0$. Thus α is an odd function and vanishes at the boundary.
Thus, if we restrict to even and odd subspaces we obtain

$$P\psi = -\psi \qquad\qquad \psi(0) = 0 = \psi(\pi), \tag{4.25}$$

or

$$P\psi = \psi \qquad\qquad (D\psi)(0) = 0 = (D\psi)(\pi), \tag{4.26}$$

and we can only get back Neumann or Dirichlet boundary conditions. Since $\alpha(0) = 0$ we do not even get mixed Neumann or Dirichlet boundary condi-

tions.
Let us make some observations which will help us solve the problem. Self-adjointness has to do with conservation of probability. Local boundary conditions assert that the probability current leaving the system at each boundary point vanishes:

$$j = -i(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) \qquad j(0) = 0\,,\, j(\pi) = 0, \tag{4.27}$$

while, for non-local boundary conditions the current leaving one boundary point can be compensated by the one entering from the other side:

$$j(0) - j(\pi) = 0, \tag{4.28}$$

where the minus sign reflects the reversed orientation of the current. Moreover, non-local boundary conditions cannot be obtained from parity reduction, since currents are odd under parity transformations:

$$P\, j\, P = -\, j, \tag{4.29}$$

and as such the current at each boundary point is bound to vanish.
In order to get non-local boundary conditions we have to lift the action to the fiber and consider the combination of charge and parity transformation, say CP, rather than P solely:

$$(CP\psi)\,(x) = \bar{\psi}(-x), \tag{4.30}$$

Indeed, CP acts not only on the base manifold but also on the U(1) fiber and can reverse the orientation on both of them. The net effect is that j is even under CP, namely

$$(CP)\; j\,(CP) = \; j, \tag{4.31}$$

so that we can have non-vanishing currents at each boundary point. From the former equation we can infer that non-local boundary conditions can emerge as a consequence of charge-parity transformations.
Within local boundary conditions we are going to prove that Robin boundary

conditions:

$$\begin{cases} \phi'(0) = \nu_0\, \phi(0), \\ \phi'(\pi) = -\nu_\pi\, \phi(\pi), \end{cases} \tag{4.32}$$

can be generated by means of parity reduction, as long as we consider the Levi-Civita connection rather than a gauge connection (compare with equation (4.20)).

We will prove that by changing the metric only in a small boundary layer we can get Robin boundary conditions starting from Neumann boundary conditions.

The relevant quantities in our problem are the spatial metric,

$$\mathrm{d}s^2 = \mathrm{d}x^2, \tag{4.33}$$

and the Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{4.34}$$

defined on $D(H_+) = \{\psi \in H^2[0,\pi] : \psi'(0) = 0 = \psi'(\pi)\}$ with Neumann boundary conditions.

Consider the following change of coordinates on the interval $[0,\pi]$:

$$x \mapsto y = F(x) \qquad y = F(x) = \int_0^x f(t)\mathrm{d}t, \tag{4.35}$$

where f is a positive function on $[0,\pi]$, such that $\int_0^\pi f(t)\mathrm{d}t = \pi$. It is easy to see that this change of coordinates leaves the endpoints of the interval unchanged, while the metric reads

$$\mathrm{d}s^2 = \left(\frac{\mathrm{d}x}{\mathrm{d}y}\right)^2 \mathrm{d}y^2 = \frac{1}{[f(y)]^2}\mathrm{d}y^2. \tag{4.36}$$

The new wavefunction ϕ changes according to the unitary transformation:

$$U_f : L^2((0,\pi),\mathrm{d}x) \to L^2((0,\pi),\mathrm{d}y), \tag{4.37}$$

$$\phi(y) = (U_f\,\psi)(y) = \frac{1}{\sqrt{g(y)}}\psi(F^{-1}(y)), \qquad g(y) = f(F^{-1}(y)), \tag{4.38}$$

because, from a local point of view, a local change of coordinates cannot change the probability: $|\psi|^2 \mathrm{d}\, x = |\phi|^2 \mathrm{d}\, y$. Under this unitary transformation, the momentum operator $p = -i\hbar\, \mathrm{d}/\mathrm{d}x$ becomes

$$p_f = U_f\, p\, U_f^\dagger = gp - \frac{i\hbar}{2} g'. \tag{4.39}$$

Accordingly, the transformed Hamiltonian reads

$$H_f = U_f\, H\, U_f^\dagger = -g^2 \frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}y^2} - gg' \frac{\hbar^2}{m} \frac{\mathrm{d}}{\mathrm{d}y} + V, \tag{4.40}$$

where

$$V = \frac{\hbar^2}{8m} \left[(g')^2 + 2gg'' \right]. \tag{4.41}$$

Next we would like to understand how the Neumann boundary conditions change under this coordinate transformation. In order to do so we compute the first derivative of $\psi(x) = \sqrt{f(x)}\phi(y(x))$:

$$\psi'(x) = \frac{1}{2\sqrt{f(x)}} f'(x)\, \phi(F(x)) + f(x) \sqrt{f(x)} \phi'(F(x)). \tag{4.42}$$

Then, at the boundary, where the functions have to vanish, we find that

$$\phi'(F(x)) = -\frac{1}{2[f(x)]^2} f'(x) \phi(F(x)), \tag{4.43}$$

that is to say

$$\begin{cases} \phi'(0) = \nu_0\, \phi(0), \\ \phi'(\pi) = -\nu_\pi\, \phi(\pi), \end{cases} \tag{4.44}$$

where $\nu_0 = -\frac{1}{2} \frac{f'(0)}{[f(0)]^2}$, $\nu_\pi = \frac{1}{2} \frac{f'(\pi)}{[f(\pi)]^2}$ and where we used the relations: $y(0) = 0$ and $y(\pi) = \pi$.

By a change of coordinates, as in equation (4.35), we managed to induce Robin boundary conditions starting from Neumann boundary conditions. However, also the original physical problem—a free quantum particle in a one-dimensional box—was changed, since, after the transformation in equation (4.38) we obtained a new Hamiltonian (4.40) with a varying mass and

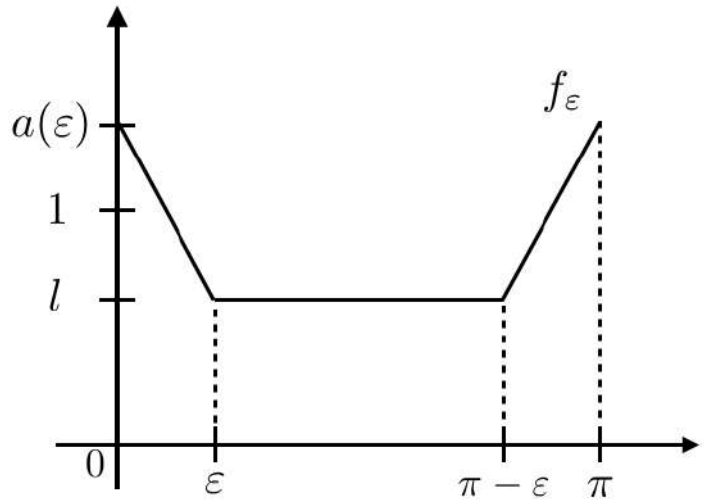

Figure 4.2: Plot of the functions f_ε, defined in(4.48), which are used for generating Robin boundary conditions.

a potential energy term $V(y)$.
In order to overcome this drawback, we will consider a sequence of functions $f_\varepsilon(x)$, $\varepsilon > 0$, which tends to a constant function in the limit $\varepsilon \to 0$, namely $f_\varepsilon(x) \to k$, pointwise for all $x \in (0, \pi)$. In principle k may even diverge, but, as we are going to see in the following, this would represent an unphysical situation. With this assumption the Hamiltonian H_{f_ε} in equation (4.40), converges in the bulk to the free particle Hamiltonian, with a renormalized mass $M = m/k^2$, that is

$$H_{f_\varepsilon} \to -\frac{\hbar^2}{2m} k^2 \frac{\mathrm{d}^2}{\mathrm{d}y^2} = -\frac{\hbar^2}{2M} \frac{\mathrm{d}^2}{\mathrm{d}y^2}. \tag{4.45}$$

Moreover we suppose that the following limits for the ε-dependent Robin constants exist:

$$\lim_{\varepsilon \to 0} \nu_0 = \mu_0 > 0, \tag{4.46}$$
$$\lim_{\varepsilon \to 0} \nu_\pi = \mu_\pi > 0. \tag{4.47}$$

For example, consider the following change of coordinates as shown in fig-

ure 4.3:

$$f_\varepsilon(x) = \begin{cases} \frac{(l-a)x}{\varepsilon} + a & 0 \leq x \leq \varepsilon, \\ l & \varepsilon \leq x \leq \pi - \varepsilon, \\ a - \frac{(l-a)(x-\pi)}{\varepsilon} & \pi - \varepsilon \leq x \leq \pi. \end{cases} \tag{4.48}$$

where $l = \frac{\pi - \varepsilon a}{\pi - \varepsilon}$ is such that $\int_0^\pi f_\varepsilon = \pi$ for every $\varepsilon > 0$ and $a = a(\varepsilon)$ is a function of ε. The Robin parameter at $x = 0$, say ν_0, reads

$$\nu_0 = -\frac{1}{2}\frac{f_\varepsilon'(0)}{[f_\varepsilon(0)]^2} = \frac{\pi}{2a^2\varepsilon}\left(\frac{a-1}{\pi - \varepsilon}\right). \tag{4.49}$$

If $a(\varepsilon) = 1/2\mu_0\varepsilon$, then in the limit $\varepsilon \downarrow 0$, the constant ν_0 converges to the fixed parameter μ_0. Interestingly, in the bulk f_ε converges to the value $\frac{2\mu_0\pi - 1}{2\mu_0\pi}$. Thus, in the interior of $(0, \pi)$, the Hamiltonian in equation (4.40) converges to the Hamiltonian of a free particle, with a renormalized mass $M = m\left(\frac{2\mu_0\pi}{2\mu_0\pi - 1}\right)^2$:

$$H_{f_\varepsilon} \to -\frac{\hbar^2}{2m}\left(\frac{2\mu_0\pi - 1}{2\mu_0\pi}\right)^2 \frac{\mathrm{d}^2}{\mathrm{d}y^2} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}y^2}. \tag{4.50}$$

If $a(\varepsilon)$, instead, diverges more slowly than $1/\varepsilon$ (and does not converge to 1), then the constant ν_0 converges to 0, that is to say to a Dirichlet boundary condition at 0. In this case, the limiting Hamiltonian in the bulk is that of a free particle with mass m

$$H_{f_\varepsilon} \to -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}y^2}, \tag{4.51}$$

because the height l converges to 1 as $\varepsilon \downarrow 0$.

Finally, if $a(\varepsilon) \to 1$, we find the Hamiltonian of a free particle with Neumann boundary conditions, as we could have expected from the very beginning. On the other hand, if $a(\varepsilon)$ diverges faster than $1/\varepsilon$ as $\varepsilon \downarrow 0$ we get an unphysical limit. In this situation, indeed, the height l diverges, which corresponds to a vanishing mass limit of the Hamiltonian in equation (4.40).

So far we have considered only what happens at $x = 0$. Analogously one can discuss the case for the other endpoint of the interval, say $x = \pi$, getting the

same results obtained for $x = 0$, say $\mu_0 = \mu_\pi$. In order to get different Robin parameters it is sufficient to consider at $x = \pi$ a value different from $a(\varepsilon)$, and then repeat the previous procedure.

4.4 Generation of boundary conditions by folding

In the previous sections we have shown how to generate quantum boundary conditions by means of a quotient procedure on the base manifold. By taking the quotient of a manifold without boundary (e.g. the circle) with respect to the action of a finite group (e.g. $\mathbb{Z}_2$), we have obtained a manifold with boundary (e.g. the interval). Then we have considered the L^2 space over the original manifold and taken a subspace (e.g. the space of even/odd wave functions) which is invariant under the action of the Hamiltonian (e.g. the Laplacian) and can be identified with the L^2 space over the quotient manifold. Thus a projection of the original quantum dynamics onto that subspace has provided the quantum dynamics on the manifold with boundary, equipped with specific quantum boundary conditions (e.g. Neumann/Dirichlet).
In the following sections we are going to show how to generate quantum boundary conditions by means of a folding procedure. At variance with the previous strategy, here we will establish a unitary map, instead of a projection, between suitable L^2 spaces over the original and the folded base manifolds. We will show that the requirement of unitarity implies the emergence of an additional spin degree of freedom in the quantum dynamics on the manifold with boundary.
In this section we consider the folding of a line into a half-line, and in the following section we will consider again the case of a circle. As a starting operator we will always take the momentum operator, which does not have self-adjoint realizations on the half-line and on the interval (with local boundary conditions), and thus cannot generate unitary dynamics. We will show how the emerging spin degree of freedom will be of help to restore unitarity.

Consider the momentum operator on the real line,

$$p = -i\hbar \frac{\mathrm{d}}{\mathrm{d}x}, \tag{4.52}$$

defined on its domain of self-adjointness,

$$D(p) = H^1(\mathbb{R}) = \{\psi \in L^2(\mathbb{R}) \mid \psi' \in L^2(\mathbb{R})\}, \tag{4.53}$$

where $H^1(\mathbb{R})$ is the first Sobolev space, of square integrable functions with square-integrable distributional derivative.

Let $\mathbb{R}_+ = \{x \in \mathbb{R} : x \geq 0\}$ be the positive half-line. We are going to construct a natural unitary map between $L^2(\mathbb{R})$ and $L^2(\mathbb{R}_+) \otimes \mathbb{C}^2$. Next, we will use this map to find out the operator on $L^2(\mathbb{R}_+) \otimes \mathbb{C}^2$ into which the original momentum operator on $L^2(\mathbb{R})$ is transformed. This procedure maps a self-adjoint operator in $L^2(\mathbb{R})$ into a self-adjoint operator in $L^2(\mathbb{R}_+) \otimes \mathbb{C}^2$. This fact is extremely interesting from a physical perspective, because, as mentioned above, the momentum operator admits no self-adjoint extensions on the half-line, say on $L^2(\mathbb{R}_+)$, since there is a net probability flux through the boundary at the origin, which cannot be compensated [RS75].

The above procedure, neverthless, will produce a self-adjoint momentum operator on the half-line at the price of the introduction of an ancillary space, $\mathbb{C}^2$. Such an operator can be physically interpreted as a Dirac operator for a spin-1/2 particle on the half-line $\mathbb{R}_+$.

We define the map

$$\begin{aligned} U : L^2(\mathbb{R}) &\to L^2(\mathbb{R}_+) \otimes \mathbb{C}^2, \\ \psi(x) &\mapsto \Phi(y) = \begin{pmatrix} \phi_+(y) \\ \phi_-(y) \end{pmatrix} = (U\psi)(y) = \begin{pmatrix} \psi(y) \\ \psi(-y) \end{pmatrix}. \end{aligned} \tag{4.54}$$

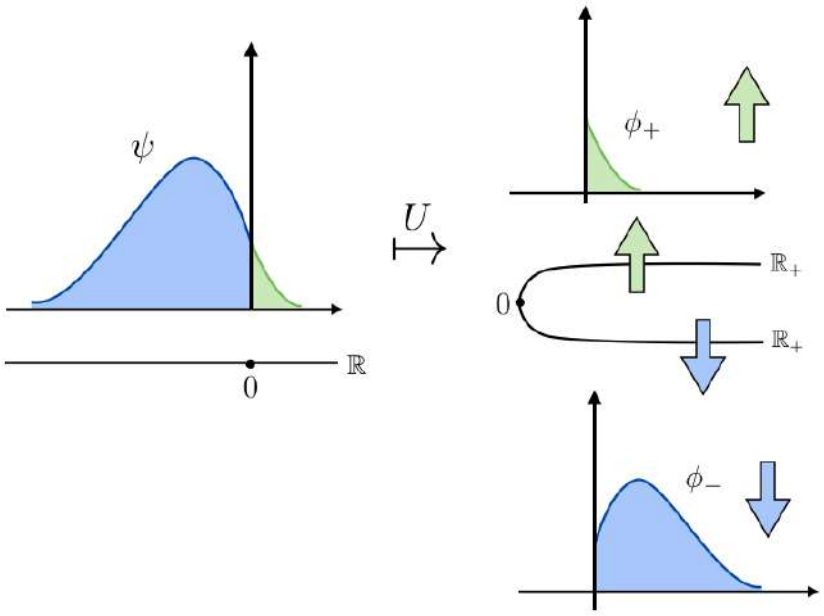

Figure 4.3: Action of the unitary operator U defined in (4.54). The splitting of the wavefunction ψ into the two spinorial components, ϕ_+ and ϕ_-, is represented.

where $x \in \mathbb{R}$ and $y \in \mathbb{R}_+$. Its adjoint reads

$$\begin{aligned} U^\dagger : L^2(\mathbb{R}_+) \otimes \mathbb{C}^2 &\rightarrow L^2(\mathbb{R}), \\ \Phi(y) = \begin{pmatrix} \phi_+(y) \\ \phi_-(y) \end{pmatrix} &\mapsto \psi(x) = (U^\dagger \Phi)(x) = \begin{cases} \phi_+(x) & \text{if } x \in \mathbb{R}_+ \\ \phi_-(-x) & \text{if } x \in \mathbb{R}_- \end{cases} \end{aligned} \tag{4.55}$$

It can be easily verified that U is unitary, namely $UU^\dagger = U^\dagger U = \mathbb{I}$.
Since the wave functions ψ in $D(p) = H^1(\mathbb{R})$ are continuous, one has that $\psi(0^+) = \psi(0^-)$. Therefore, the domain of the transformed operator $\tilde{p} = UpU^\dagger$ is

$$D(\tilde{p}) = UD(p) = \{\Phi \in H^1(\mathbb{R}_+) \otimes \mathbb{C}^2 \,|\, \phi_+(0) = \phi_-(0)\}. \tag{4.56}$$

It is clear from the above expression that a boundary condition has naturally emerged after this unitary transformation.

Let us now look at the explicit form of the operator $\tilde{p} = UpU^\dagger$. We get

$$\begin{aligned}(pU^\dagger\Phi)(x) = pU^\dagger \begin{pmatrix}\phi_+\\ \phi_-\end{pmatrix}(x) &= p\begin{cases}\phi_+(x) & \text{if } x\in\mathbb{R}_+\\ \phi_-(-x) & \text{if } x\in\mathbb{R}_-\end{cases}\\ &= -i\hbar\begin{cases}\phi'_+(x) & \text{if } x\in\mathbb{R}_+\\ -\phi'_-(-x) & \text{if } x\in\mathbb{R}_-\end{cases},\end{aligned} \tag{4.57}$$

whence

$$\tilde{p}\Phi(y) = UpU^\dagger \begin{pmatrix}\phi_+(y)\\ \phi_-(y)\end{pmatrix} = -i\hbar\begin{pmatrix}\phi'_+(y)\\ -\phi'_-(y)\end{pmatrix}. \tag{4.58}$$

Therefore,

$$\tilde{p} = -i\hbar\frac{\mathrm{d}}{\mathrm{d}y}\otimes\sigma_z \qquad D(\tilde{p}) = \{\Phi\in H^1(\mathbb{R}_+)\otimes\mathbb{C}^2\,|\Phi(0) = \sigma_x\Phi(0)\,\}, \tag{4.59}$$

where σ_x and σ_z are the first and the third Pauli matrix, respectively.
In words, we started with the momentum operator p of a quantum particle on the line $L^2(\mathbb{R})$. Then, we punctured the line at the origin and folded it, resulting into two copies of $L^2(\mathbb{R}_+)$, that is $L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$. See Fig. 4.3. Next, we showed that the momentum on the real line transforms into a Dirac operator on the half-line with a definite quantum boundary condition which makes it self-adjoint.
It is instructive to look at the above procedure in the opposite way, which would represent a dilation process: Suppose we start with the momentum operator on the half-line, i.e. in $L^2(\mathbb{R}_+)$, which admits no self-adjoint extensions, because its deficiency indices are different [RS75]. Then, instead of giving up, in the spirit of Naimark's dilation theorem [AG93], one can instead enlarge the Hilbert space and look at an extension of the problem one has started with, which is significantly different. In other words, through a dilation procedure, we can get the operator $\tilde{p}$, which is a Naimark extension of the momentum on the half-line and has a different physical interpretation, as the Dirac operator of a spin-1/2 particle on the half-line.

From a physical point of view the new operator $\tilde{p}$ could represent a spin-1/2 particle interacting with a wall, which flips both the momentum and the spin of the particle, through the operator σ_x in the boundary conditions (4.59), and thus preserves its helicity. An alternative interpretation is given by a spinless particle on the half-line which collides with a detector at the boundary. The detector has two possible states and corresponds to the two-level system. When the particle hits the boundary, it will bounce with a corresponding flip of its momentum, and the detector will click.
More generally one can consider the momentum operator for a free particle on a punctured line. In this case we are adding a delta-like potential in a point on the line, which is responsible for a phase-shift of order $\mathrm{e}^{i\alpha}$, $\alpha \in \mathbb{R}$, in the wavefunction when the particle reaches the potential. The operator reads:

$$p_\alpha = -i\hbar \frac{\mathrm{d}}{\mathrm{d}x} \oplus -i\hbar \frac{\mathrm{d}}{\mathrm{d}x}, \tag{4.60}$$

$$D(p_\alpha) = \{\psi \in H^1(\mathbb{R}_+) \oplus H^1(\mathbb{R}_-) \,:\, \psi(0^-) = \mathrm{e}^{i\alpha}\psi(0^+)\}. \tag{4.61}$$

After the folding process by means of the unitary operator U in equation (4.54) the transformed operator on the half-line becomes:

$$\tilde{p}_\alpha = -i\hbar \frac{\mathrm{d}}{\mathrm{d}y} \otimes \sigma_z \qquad D(\tilde{p}_\alpha) = \{\Phi \in H^1(\mathbb{R}_+) \otimes \mathbb{C}^2 \,|\, \phi_-(0) = \mathrm{e}^{i\alpha}\phi_+(0)\,\}. \tag{4.62}$$

Then, the boundary conditions become:

$$\phi_-(0) = \mathrm{e}^{i\alpha}\phi_+(0) \iff \begin{pmatrix}\phi_+(0)\\ \phi_-(0)\end{pmatrix} = \left(\cos\alpha\,\sigma_x + \sin\alpha\,\sigma_y\right)\begin{pmatrix}\phi_+(0)\\ \phi_-(0)\end{pmatrix}. \tag{4.63}$$

The above boundary conditions can be recast in a more compact form by considering the phase α as an angle in the xy plane, namely equation (4.63) can be rewritten as:

$$\Phi(0) = (n \cdot \sigma)\Phi(0), \tag{4.64}$$

$n = (\cos\alpha, \sin\alpha)$ being a unitary vector lying in the xy plane and $\sigma = (\sigma_x, \sigma_y)$. Summing up we have found that the folded operator on the half-

line reads:

$$\tilde{p}_\alpha = -i\hbar\frac{\mathrm{d}}{\mathrm{d}y}\otimes\sigma_z \qquad D(\tilde{p}_\alpha) = \{\Phi \in H^1(\mathbb{R}_+)\otimes\mathbb{C}^2 \,|\, \Phi(0) = (n\cdot\sigma)\Phi(0)\}.$$

$$n = (\cos\alpha, \sin\alpha) \tag{4.65}$$

Thus, while the Dirac operator is always σ_z, the boundary conditions can be changed and handled on the orthogonal xy plane .

4.5 Entanglement generation and self-adjointness

There is an increasing interest in the connection between boundary conditions and entanglement generation [IMP14].
In the previous section manifestly we proved that the self-adjointness of the resulting operator relied on the introduction of an ancillary spin.
Indeed, the dynamics on the space $L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$ is unitary, but this cannot be the case on the spatial component $L^2(\mathbb{R}_+)$, since its generator, the momentum operator, is not self-adjoint on the half-line. The momentum operator on the line is not projectable onto the half-line, and this results in the projected operator losing self-adjointness.
This issue can be detected by considering the projection of the space $L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$, which is unitarily equivalent to $L^2(\mathbb{R})$, onto its spatial component $L^2(\mathbb{R}_+)$. This projection, obtained by tracing out the spin component $\mathbb{C}^2$, maps separable pure states into pure states, while entangled states are mapped into mixed states. Therefore, if the unitary dynamics on $L^2(\mathbb{R}_+)\otimes\mathbb{C}^2$ generates entanglement, its projection cannot be unitary. This establishes an interesting link between entanglement generation of a unitary evolution and the lack of self-adjointness of the projected generator.
That is just the case of the example under consideration. Indeed, suppose that the system is initially in the factorized state:

$$\phi\otimes\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}, \tag{4.66}$$

where $\phi \in L^2(\mathbb{R}_+)$ is a normalized wave packet which vanishes in a neighbourhood of the origin $x = 0$, and $\{|\uparrow\rangle, |\downarrow\rangle\}$ is the eigenbasis of σ_z. Then, the evolved state for sufficiently small times reads:

$$e^{-itp\otimes\sigma_z}\left(\phi(x)\otimes\frac{|\uparrow\rangle+|\downarrow\rangle}{\sqrt{2}}\right)=\phi(x-t)\otimes\frac{|\uparrow\rangle}{\sqrt{2}}+\phi(x+t)\otimes\frac{|\downarrow\rangle}{\sqrt{2}}, \tag{4.67}$$

and the spatial degrees of freedom get manifestly entangled with the spinorial ones for positive times.

Thus, we notice how the dynamics induced by the self-adjoint operator $\tilde{p}$ generates entanglement on the half-line. Interestingly, one could generate entanglement differently. Indeed, suppose the system is initially in the state:

$$\phi\otimes|\downarrow\rangle, \tag{4.68}$$

$\phi \in L^2(\mathbb{R}_+)$, then one could think that its evolved state at a later time t, would be:

$$\phi(x+t)\otimes|\downarrow\rangle, \tag{4.69}$$

and, as such, should not be entagled. This is not true. Indeed, equation (4.69) holds as long as the wave packet ϕ does not collide with the boundary. When the wavepacket collides with the boundary, part of the original spin up component gets transformed into a spin down component, so that the overall evolved state gets entangled, namely:

$$\phi(-x+t)\theta(-x+t)\otimes|\uparrow\rangle+\phi(x+t)\theta(x+t)\otimes|\uparrow\rangle. \tag{4.70}$$

For large enough times, thus, although starting from a factorized state, whose spin component should be left invariant by the overall evolution because $|\downarrow\rangle$ is an eigenstate of σ_z, we have a generation of entanglement due to the presence of th boundary. Indeed, it is due to the boundary conditions that spin up and spin down components get mixed up and, as a result, entanglement is generated.

More generally, if we start from a state $\Phi = \phi_+ \otimes |\uparrow\rangle + \phi_- \otimes |\downarrow\rangle$, then the

evolved state reads:

$$\left(e^{-itp\otimes\sigma_z}\Phi\right)(x) = \begin{pmatrix} \phi_+(x-t)\theta(x-t) + \phi_-(-x+t)\theta(-x+t) \\ \phi_+(-x-t)\theta(-x-t) + \phi_-(x+t)\theta(x+t) \end{pmatrix}. \quad (4.71)$$

where x is a coordinate of $\mathbb{R}_+$. As a final comment, we remark that the folding procedure admits regions where the dynamics is and keeps on being separable. For example, if we start with a state $\phi \otimes |\uparrow\rangle, \phi \in L^2(\mathbb{R}_+)$, then, from equation (4.71) we get that the evolved state will stay separable for any time $t > 0$, since the evolved state is: $\phi(x-t) \otimes |\uparrow\rangle$. In the previous case, in fact, it was the crossing of the boundary that generated entanglement.

If one starts with a non separable state and evolve for a short time, then, entanglement will be generated due to the evolution of the system (compare with equation (4.67)). As a result, the evolved state, when projected on the half-line, becomes a mixed state.

This procedure of entanglement generation can be explained in terms of the non projectability of the momentum operator on the half-line.

Indeed, we could compare what happens when the dynamics is generated by the square of $\tilde{p}^2 = Up^2U^\dagger$, which is nothing but the folded Laplacian operator, say:

$$\tilde{p}^2 = -\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}^2 y} \otimes \mathbb{I} \quad (4.72)$$

$$D(\tilde{p}^2) = \{\Phi \in H^2(\mathbb{R}_+) \otimes \mathbb{C}^2 \,|\Phi(0) = \sigma_x\Phi(0)\,,\, \Phi'(0) = -\sigma_x\Phi'(0)\,\}, \quad (4.73)$$

where $\Phi'(0) = (\phi'_+(0), \phi'_-(0))$. As we are going to check this operator admits states which are projectable at any time.

Indeed, if the initial state is $\phi \otimes (|\uparrow\rangle + |\downarrow\rangle)$, $\phi \in L^2(\mathbb{R}_+)$, then the evolved state will stay factorized and it will be of the form $\phi_t \otimes (|\uparrow\rangle + |\downarrow\rangle)$, where $\phi_t = \mathrm{e}^{-\mathrm{ip}^2\mathrm{t}}\phi$.

Vectors of the form $\phi \otimes (|\uparrow\rangle + |\downarrow\rangle)$ correspond to even functions on the real line, as it can be proved with the operator U in equation (4.54).

Indeed, the parity operator $P : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, $(P\psi)(x) = \psi(-x)$, on the

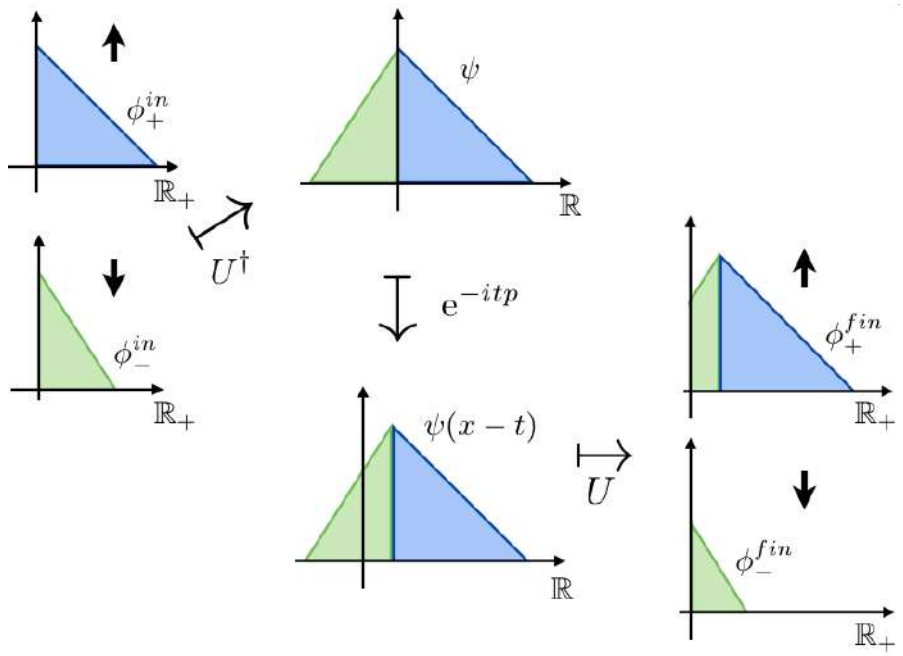

Figure 4.4: Graphical representation of equation (4.71). We start our evolution with the state $\Phi = (\phi_+^{in}, \phi_-^{in})$. By means of $U^\dagger$ we unfold Φ on the real line. The system evolves under the operator p, and eventually we fold it back into the spinor $(\phi_+^{fin}, \phi_-^{fin})$.

folded space reads:

$$\tilde{P}\Phi = (UPU^\dagger) \begin{pmatrix} \phi_+(y) \\ \phi_-(y) \end{pmatrix} = \sigma_x \begin{pmatrix} \phi_+(y) \\ \phi_-(y) \end{pmatrix}, \tag{4.74}$$

Thus $\tilde{P}$ commutes with the boundary conditions, namely σ_x and, for this reason, cannot create entanglement on the subspace generated by the set of even functions. Thus, factorized states, which emerge from even functions, get projected into pure states. Analogously follows for odd functions, which correspond to states of the form $\phi \otimes (|\uparrow\rangle - |\downarrow\rangle)$
Differently, if we start, for example, with a state $\phi \otimes |\uparrow\rangle$, $\phi \in L^2(\mathbb{R}_+)$, although factorized, it will entangle. Moreover, notice that the dynamical generation of entanglement is due to the boundary condition which emerged in the folding process.

4.6 Momentum operator on the circle

In this section we would like to provide the reader with another example of the folding procedure. We are going to study the momentum of a particle on a circle $\mathbb{S}$ and, alike the previous section, we will map this problem into a unitarily equivalent one. As a consequence, boundary conditions will be generated in the transformed system.
We recall the natural identifications:

$$L^2(\mathbb{S}) = L^2(-\pi,\pi) = L^2(-\pi,0) \oplus L^2(0,\pi), \tag{4.75}$$

that will turn out to be useful in the following discussion. Consider the momentum operator of a particle on a circle

$$p = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}, \qquad D(p) = H^1(\mathbb{S}) = \{\psi \in H^1[-\pi,\pi] \mid \psi(-\pi) = \psi(\pi)\,\}. \tag{4.76}$$

By using the identifications (4.75) and the continuity of the functions in the first Sobolev space H^1, the domain of p can be rewritten as

$$D(p) = \{\psi \in H^1[-\pi,0] \oplus H^1[0,\pi] \mid \psi(0^-) = \psi(0^+)\,,\, \psi(-\pi) = \psi(\pi)\}. \tag{4.77}$$

We are going to unitarily map this problem on $L^2(0,\pi)\otimes\mathbb{C}^2$. Indeed the following map is unitary, as pictorially shown in figure 4.5:

$$U : L^2(\mathbb{S}) \;\to\; L^2(0,\pi)\otimes\mathbb{C}^2, \tag{4.78}$$

$$\psi(x) \;\mapsto\; (U\psi)(y) = \begin{pmatrix}\phi_+(y)\\ \phi_-(y)\end{pmatrix} = \begin{pmatrix}\psi(y)\\ \psi(-y)\end{pmatrix}, \tag{4.79}$$

where $x \in [-\pi,\pi]$ and $y \in [0,\pi]$. Its inverse reads

$$U^\dagger : L^2(0,\pi)\otimes\mathbb{C}^2 \;\to\; L^2(\mathbb{S}),$$

$$U^\dagger \begin{pmatrix}\phi_+(y)\\ \phi_-(y)\end{pmatrix} = \begin{cases}\phi_+(x) & \text{if } x \in [0,\pi]\\ \phi_-(-x) & \text{if } x \in [-\pi,0]\end{cases}. \tag{4.80}$$

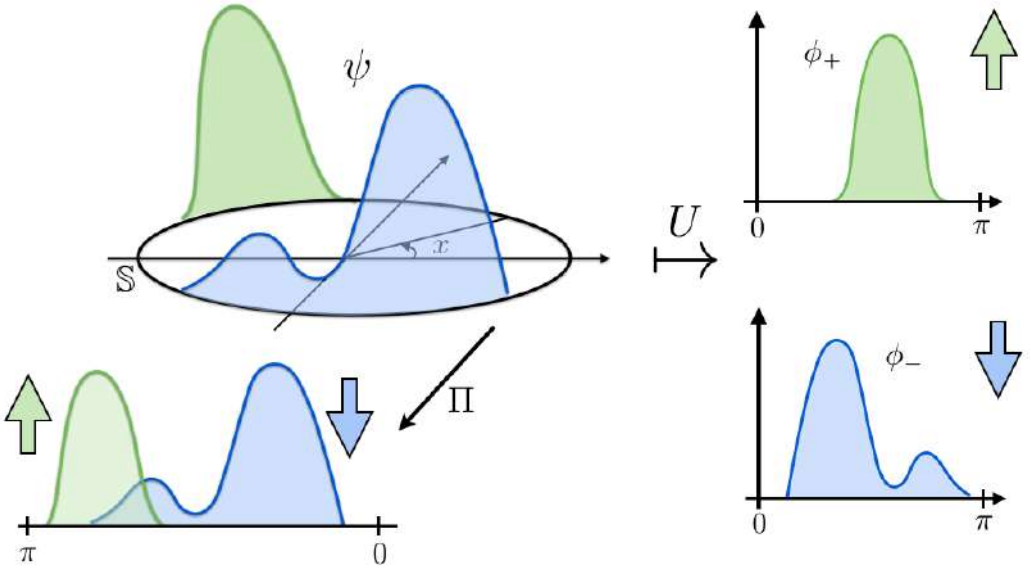

Figure 4.5: Action of the unitary operator U on $L^2(\mathbb{S})$ defined in (4.86). The splitting of the wavefunction ψ into the two spinorial components, ϕ_+ and ϕ_-, is represented (on the right). On the left the folding procedure on the interval $[0, \pi]$ is pictorially shown.

The domain of the transformed operator $\tilde{p} = UpU^\dagger$ is

$$D(\tilde{p}) = UD(p) = \{\Phi \in H^1[0,\pi] \otimes \mathbb{C}^2 \,|\, \phi_+(0) = \phi_-(0)\,,\, \phi_+(\pi) = \phi_-(\pi)\}. \tag{4.81}$$

and $\tilde{p}$ acts as

$$\tilde{p} \begin{pmatrix} \phi_+(y) \\ \phi_-(y) \end{pmatrix} = -i\hbar \begin{pmatrix} \phi'_+(y) \\ -\phi'_-(y) \end{pmatrix}. \tag{4.82}$$

Therefore, we get

$$\tilde{p} = -i\frac{\mathrm{d}}{\mathrm{d}y} \otimes \sigma_z, \tag{4.83}$$

$$D(\tilde{p}) = \{\Phi \in H^1[0,\pi] \otimes \mathbb{C}^2 \,|\Phi(0) = \sigma_x\,\Phi(0)\,,\, \Phi(\pi) = \sigma_x\,\Phi(\pi)\}. \tag{4.84}$$

In a nutshell, we started from the momentum operator on the unit circle and by means of a unitary transformation we ended up with the Dirac operator on a segment with well-prescribed boundary conditions.

As in the previous example, we managed to obtain a spin-1/2 particle on a manifold with boundary starting from a spinless particle on a manifold without boundary. Again, the emergent spin degrees of freedom are crucial in the conservation of probability, since the quantum boundary conditions imply both a spin flip and a momentum flip whenever the particle bounces off the boundary.

Let us conclude this section with some comments comparing the reduction and folding procedures. Let us fix our attention on even and odd functions on the circle. Under the action of the unitary operator U in equation (2.2) an even function on the circle, say ψ, transforms into:

$$\begin{aligned} \psi(x) \mapsto (U\psi)(y) &= \begin{pmatrix} \psi(y) \\ \psi(-y) \end{pmatrix} = \begin{pmatrix} \psi(y) \\ \psi(y) \end{pmatrix} = \psi(y) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \\ &= \sqrt{2}\psi \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \end{aligned} \tag{4.85}$$

Then, when we trace out on the spin degrees of freedom we find the results of the reduction procedure. Indeed, in the projection procedure, pure states (which originate from even functions on the circle) are mapped in pure states because the square operator of $\tilde{p}^2 = -\hbar^2 \mathrm{d}^2/\mathrm{d}^2 y \otimes \mathbb{I}$ is projectable. For this reason, if we focus our attention on suitable subspaces, e.g. even or odd functions, the dynamics cannot generate entanglement, because the projected operator as well is self-adjoint.

Thus, the reduction procedure can be obtained from the folding one when the spin degrees of freedom are traced out. In fact, whenever this procedure is admissible we find that the operator is projectable because it admits eigensubspaces which are left invariant by the action of a group action, e.g. the parity action. In particular, the condition $[H, P] = 0$ guarantees for the operator H to be projectable with respect to the quotient.

The folding procedure, instead, is more general since it does not require any compatibility relation between the operator and a group action.

4.7 Naimark's theorem and generalizations

In this section we would like to discuss with more details the construction discussed in the previous section by means of Naimark's theorem [AG93]. First of all we recall what we mean by deficiency indices of a symmetric operator. Let A be a symmetric operator and A^* its adjoint (see chapter 5). The deficiency subspaces of A are $K_\pm = N(A^* \pm iI)$, and the relative dimensions say $n_\pm = \dim K_\pm$ are called the deficiency indices of the operator A. As a matter of fact they quantify the lack of self-adjointness of a symmetric operator, as quantitatively discussed by von Neumann theorem's on self-adjoint extensions [Neu55]:

Theorem 2. *Let A be a symmetric operator, whose deficiency indices are n_+ and n_-. Then, A admits self-adjoint extensions if and only if $n_+ = n_-$. Moreover there is a 1-1 correspondence between self-adjoint extensions of A and unitary operators between K_- and K_+ (infinite extensions if $n_+ = n_- \geq 1$; one and only one if $n_+ = n_- = 0$).*

For example the Hamiltonian operator describing a free quantum particle on a segment $(0, 1)$, say:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \quad , \quad D(H) = C_0^\infty(0,1) \tag{4.86}$$

has deficiency indices $n_\pm = 2$, and for this reason it admits infinitely many self-adjoint extensions, which have already been discussed in section 1.6. Differently, the momentum operator on the half-line, say on $L^2(\mathbb{R}_+)$:

$$p_0 = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x} \qquad D(p_0) = H_0^1(\mathbb{R}_+) = \{\psi \in H^1(\mathbb{R}_+) \,:\, \psi(0) = 0\}, \tag{4.87}$$

admits no self-adjoint extension, because $n_+ = 1 \neq n_- = 0$, and cannot be used to represent a physical observable. This can be easily explained physically if one invokes the principle of conservation of probability. As a matter of fact, the evolution of a closed quantum system is unitary and there cannot be a net loss of probability for the whole evolution time. In our

case, when the particle scatters against the wall, say at the point 0, part of the probability density associated to it passes through the wall, causing a loss of probability. As a result, we would expect this missing part to return somehow, from the other side of the half-line. Of course, this cannot happen and, as such, the operator p cannot represent a physical observable, admitting no self-adjoint extension.
Nevertheless, as we are going to discuss, it admits other kind of extensions, as provided by Naimark's theorem. Indeed, we are going to prove that extensions can always be built up on a larger space:

Every symmetric operator A in a Hilbert space $\mathscr{H}$ has a minimal extension in $\mathscr{H} \otimes \mathbb{C}^2$.

Before discussing this result we quickly recall the Naimark theorem [AG93], which states that:

Theorem 3. *Every symmetric operator A defined on a Hilbert space $\mathscr{H}$ with arbitrary deficiency indices, (n_+, n_-), can be extended to a self-adjoint operator B, defined on a larger Hilbert space $\mathscr{H}^+ \supset \mathscr{H}$.*

As a matter of fact, the operator B can be manifestly constructed from A. Indeed one can choose a Hilbert space $\mathscr{H}'$ isomorphic to $\mathscr{H}$ by means of a unitary operator $U : \mathscr{H} \to \mathscr{H}'$ and build an operator A' with reversed deficiency indices, namely (n_-, n_+), for example $A' = -UAU^\dagger$.
Then, define $\mathscr{H}^+ = \mathscr{H} \oplus \mathscr{H}'$ and $A^+ = A \oplus A'$. Manifestly A^+ extends A and it is easily proved that its deficiency indices are equal $(n_+ + n_-, n_+ + n_-)$ and by the von Neumann theorem it admits self-adjoint extensions.
In light of the Naimark theorem, let us analyze the momentum operator on the half line. The adjoint of p_0 is:

$$p_0^* = -i\hbar \frac{\mathrm{d}}{\mathrm{d}x} \qquad D(p_0^*) = H^1(\mathbb{R}_+), \tag{4.88}$$

so that the deficiency indices read $(1, 0)$. Consider, now, the operator $-p_0$ on $L^2(\mathbb{R}_+)$, whose deficiency indices are $(0, 1)$. We would like to obtain an

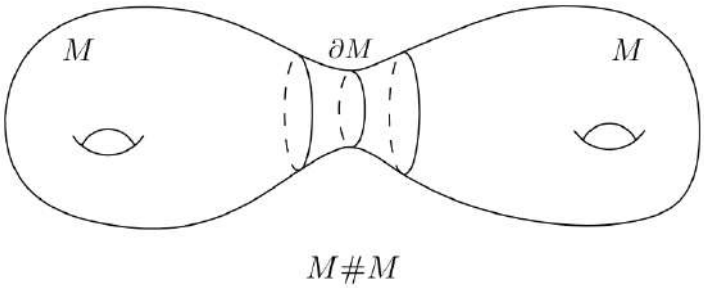

Figure 4.6: The double of a smooth manifold M.

extension on $L^2(\mathbb{R})$, and for this reason we consider the following unitary operator:

$$U : L^2(0,\infty) \to L^2(-\infty,0), \tag{4.89}$$

such that $(U\psi)(x) = \psi(-x)$. Next we define

$$p_0' = -U\, p_0 U^\dagger = -i\hbar \frac{\mathrm{d}}{\mathrm{d}x}, \tag{4.90}$$

whose deficiency indices are $(0,1)$ and whose domain is $D(p_0') = H_0^1(\mathbb{R}_-) = \{\psi \in H^1(\mathbb{R}_-) \,:\, \psi(0) = 0\}$. Then, we consider

$$\mathscr{H}^+ = L^2(\mathbb{R}) = L^2(0,\infty) \oplus L^2(-\infty,0), \tag{4.91}$$

$$p_0^+ = p_0 \oplus p_0', \tag{4.92}$$

where $D(p_0^+) = D(p_0) \oplus D(p_0') = \{\psi \in H^1(\mathbb{R}/\{0\})\,,\, \psi(0) = 0\}$ and whose deficiency indices are equal, $(1,1)$. Thus, p_0' admits self-adjoint extensions. As a corollary from the Naimark theorem it follows that:

Theorem 4. *Every symmetric operator A in $\mathscr{H}$ has a minimal extension in $\mathscr{H} \otimes \mathbb{C}^2$.*

Indeed, consider a manifold with boundary M and a symmetric operator A on $L^2(M)$. We consider the double of a smooth manifold with boundary [Lee02], denoted by $M\#M$, obtained from the disjoint union $M \bigcup M$ by identifying each boundary point in one copy of M with the same boundary point in the other. The manifold obtained is a smooth manifold without

boundary and contains two regular domains diffeomorphic to M (See Figure 4.6). Moreover suppose that A has deficiency indices (n_+, n_-). As shown in the previous discussion, one can find an operator $A' = -A$ on $L^2(M)$ with inverted deficiency indices (n_-, n_+).
Then, the operator $A \oplus A'$ is symmetric on $L^2(M\#M) \cong L^2(M) \oplus L^2(M)$, with equal deficiency indices $(n_+ + n_-, n_+ + n_-)$. Eventually, it follows by von Neumann's theorem that $A \oplus A'$ admits self-adjoint extensions on $L^2(M\#M)$.
Summing up we started from a symmetric operator on $L^2(M)$ with different deficiency indices. Apparently this operator could not admit self-adjoint extensions and we found a way to get around this problem with the introduction of an auxiliary Hilbert space. In particular, we considered the double of the base manifold M, namely $M\#M$, a manifold without boundary, where, by means of Naimark's theorem, self-adjoint extensions of the operator we started with can be built up.
This procedure enables a constructive way for realizing self-adjoint extensions of symmetric operators, which do not satisfy the hypotheses of von Neumann's theoreom.
The Hilbert space $L^2(M\#M)$ is isomorphic to two copies of $L^2(M)$ which can be unitarily recasted into another Hilbert space $L^2(M) \otimes \mathbb{C}^2$:

$$L^2(M\#M) \cong L^2(M) \oplus L^2(M) \cong L^2(M) \otimes \mathbb{C}^2. \tag{4.93}$$

The latter isomorphism shows manifestly an interesting physical interpretation, which was already discussed in the examples of section 4.4 and 4.6. Indeed, the doubling of the base space adds an additional spin degree of freedom to the system.
For example, suppose that A is a symmetric differential operator on M. The operator A may be used to describe an observable for a physical system settled in M. In particular, if its deficiency indices are different, we can implement the procedure resulting from Naimark's theorem. In light of the previous discussion, A admits a self- adjoint extension on $L^2(M) \otimes \mathbb{C}^2$, thus for a physical system admitting spin degrees of freedom. From a physical perspective the operator A can never represent an observable for the physical

system we started with. Rather its extension, by means of the Naimark's procedure, can be effectively used, but it will describe the physical system with additional spin degrees of freedom.

Let us conclude this section with an additional comment. In the previous construction we took $A' = -A$. In the case of the momentum operator we obtained two copies of the momentum operator on the half line, namely: $p_0^+ = p_0 \oplus p_0'$. The operator p_0 has deficiency indices equal to $(1, 0)$, while the operator p_0' has inverted deficiency indices, namely $(0, 1)$. If we start our evolution with spin $|\uparrow\rangle$, there will never be generation of entanglement for $t > 0$ due to p_0. Analogously the operator $-p_0$ cannot generate entangle for negative times and an initial state with spin down $|\downarrow\rangle$. Thus the position of 0 in the deficiency indices can make us understand in which direction we are creating entanglement or analogously can provide information on the loss of probability due to the lack of self-adjointness. Indeed, if we start with a spin up state and we have no entanglement generation for positive times, we will be sure that the second deficiency index is equal to 0.

Chapter 5

Quantum boundary conditions: mathematical results

In this chapter we are going to state and prove the mathematical tools used in the previous chapters. In particular, we are going to prove that the set of the self-adjoint extensions of the kinetic energy operator for a free quantum particle in a cavity is in a one-to-one correspondence with the set of unitary operators on a Hilbert space at the boundary. Moreover, we are going to compare and contrast this formulation with the ones already available in the literature [FGL17b].

5.1 Introduction

In the last few years there has been an increasing interest in the physics of quantum systems confined in a bounded spatial region and in the prominent role of quantum boundary conditions (See Chapter 1).
Several examples were analyzed, ranging from the Aharonov-Bohm effect in quantum mechanics, to the quantum Hall effect in solid state physics, from anomalies and the Casimir effect in quantum field theory, to fluctuating topologies in quantum gravity.

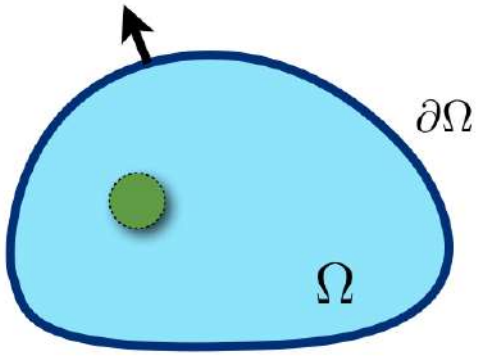

Figure 5.1: A quantum particle confined into a cavity Ω

In section 1.6 we asserted that all the physical dynamics of a closed quantum system are implemented by a strongly continuous one-parameter unitary group, which by the Stone theorem is in a one to one correspondence with its generator that must be a self-adjoint operator. See e.g. [RS75]. Physically, the generator is the system's Hamiltonian and it corresponds to the energy observable. For example, the Hamiltonian of a free nonrelativistic particle in $\mathbb{R}^n$ is just its kinetic energy and is given by

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\Delta,$$

where $\hbar$ is the Planck constant and m is the mass of the particle (In the following, for simplicity, we will set $\hbar^2/2m = 1$). H is an operator on the Hilbert space $L^2(\mathbb{R}^n)$ with domain, e.g., $D(H) = C_c^\infty(\mathbb{R}^n)$, the smooth functions of compact support. On $D(H)$ the Hamiltonian is symmetric but is not self-adjoint, whence it does not represent any physical observable, and cannot generate any physical dynamics. However, its closure $\overline{H}$ is a self-adjoint operator (i.e. H is essentially self-adjoint), and as such it represents the Hamiltonian of a free particle [RS75].

The situation drastically changes in the presence of boundaries. The kinetic energy operator of a particle in an open bounded set Ω, defined as the Laplace operator on $L^2(\Omega)$ with domain $D(H) = C_c^\infty(\Omega)$, is still symmetric but it is no more essentially self-adjoint, and as such its closure does not correspond

to any physical observable. Indeed, H admits infinite self-adjoint extensions — that is infinite possible dynamics — each one characterized by a given physical behavior of the particle at the boundary $\partial\Omega$.

This paradigmatic example explains the compelling reason, since the inception of quantum mechanics, for searching and characterizing all the self-adjoint extensions (if any) of a given symmetric operator, which is formally associated to a system on physical grounds.

The answer was soon given by von Neumann in his theory of self-adjoint extensions, which is one of the gems of functional analysis [Neu55]. This theory is fully general and completely solve the problem of self-adjoint extensions of every densely defined and closed symmetric operator in an abstract Hilbert space in terms of unitary operators between its deficiency subspaces. See e.g. [Oli08].

In order to reach its goal of encompassing all possible operators, von Neumann's theory should necessarily work at an abstract level. However, for specific classes of operators it would be desirable to have a more concrete characterization of the set of self-adjoint extensions. In particular, for differential operators on a bounded spatial region, as in the above example of the free particle, one would like to establish a direct connection between self-adjoint extensions and boundary conditions. This is highly appealing from a physical perspective, since it would allow to implement a specific dynamics by building the confining wall out of a suitable material.

A concrete characterization was given by Grubb [Gru68] for symmetric even-order elliptic differential operators in a bounded regular spatial domain. Building on the earlier work of Višik [Vis63], Birman [Bir56], and Lions and Magenes [LM72], she was able to characterize all the self-adjoint extensions in terms of boundary conditions parametrized by (unbounded) self-adjoint boundary operators $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ acting on closed (proper) subspaces $\mathcal{X}$ of the boundary Hilbert space. See Theorem 6 for the Laplace operator.

At an intermediate level of abstraction between Grubb's and von Neumann's descriptions lies the theory of boundary triples [BGP08; Oli08], which elaborates on ideas of Calkin [Cal39] and Vishik [Vis63], and is valid for every

symmetric operators, because it relies on an abstraction of the notion of boundary values in function spaces. A related description was discovered in the last years by Posilicano [Pos08], who introduced a parametrization in terms of pairs (Π, Θ), where Π is an orthogonal projection in an auxiliary Hilbert space $\mathfrak{h}$ and Θ is a self-adjoint operator in the range of Π. See also [Del15]. When particularized to differential operators, one recovers Grubb's parametrization, where $\mathfrak{h}$ is essentially the boundary space, Π is the projection onto $\mathcal{X}$ and Θ is L.

Recently, Asorey, Marmo and Ibort [AIM05; AIM15] proposed on physical ground a different parametrization of the self-adjoint extensions of differential operators in terms of *unitary* operators U on the boundary. This description relies more directly on physical intuition and in the last years it has been applied to several systems ranging from one dimensional quantum systems with changing boundary conditions [Aso+13] or with moving boundaries [Di +16; Fac+16], to the Aharonov-Bohm effect [OP10], to field theories [AGM15], and in particular to the investigation of vacuum fluctuations and the Casimir effect [AM11; AM13].

The large use of this description in several physical applications is also due to its great manageability: the parametrization is in terms of a single unitary operator U on the boundary, instead of a pair $(\mathcal{X}, L)$ composed of a closed subspace $\mathcal{X}$ and a self-adjoint operator L, which in general is unbounded and thus also needs a domain specification $D(L)$. Here, all information is encoded in a single simpler object.

This characterization is close in spirit to von Neumann's theory. However, it is different in one essential aspect: the unitaries are boundary operators, rather than bulk operators, and as such they are more directly related to experimental implementations, as discussed above. Indeed, along the same lines as [Pos03], it is possible to connect the two pictures, and to exhibit an explicit relation between the boundary and the bulk unitaries, but the result will not be very transparent.

We are going to establish a characterization of the self-adjoint extensions of an elliptic differential operator in terms of unitary operators on the boundary. In this chapter we will focus on the above-mentioned paradigmatic model of

the Laplacian in a bounded regular domain, that is the model of a free nonrelativistic particle in a box.

We will establish, in Theorem 5, a bijection between the set of self-adjoint extensions of the Laplace operator on a bounded regular domain and the set of boundary unitary operators. Each unitary operator is characteristic of a specific boundary condition, that is a relation between the boundary value, $\boldsymbol{\gamma}\psi$, of the function ψ and its normal derivative at the boundary, $\boldsymbol{\nu}\psi$, (in the sense of traces). Recall that the trace of a function in $L^2(\Omega)$ is in $H^{-1/2}(\partial\Omega)$, the Sobolev space of negative fractional order $-1/2$ [LM72]. This will be the natural arena of our boundary conditions, that is the boundary Hilbert space the unitaries U will act on.

The explicit relation, given in Remark 2, reads

$$\boldsymbol{\mu}\psi - i\boldsymbol{\gamma}\psi = U(\boldsymbol{\mu}\psi + i\boldsymbol{\gamma}\psi),$$

and, in fact, it links the boundary value $\boldsymbol{\gamma}\psi$ of the function ψ to the *regular part* $\boldsymbol{\mu}\psi$ of its normal derivative $\boldsymbol{\nu}\psi$, see Definition 5. This is consistent with a different regularity of the boundary values of the function and of its normal derivative: in general their traces belong to different Sobolev spaces, $H^{-1/2}(\partial\Omega)$ and $H^{-3/2}(\partial\Omega)$ respectively, and cannot be compared. Interestingly enough, the irregular part of the normal derivative plays no role in the boundary conditions; indeed, it is not an independent boundary datum, and indeed is completely determined by the trace of the function $\boldsymbol{\gamma}\psi$ through the Dirichlet-to-Neumann operator [Gru09].

A crucial ingredient in proving that the irregular part of the normal derivative is immaterial to the boundary conditions is the generalized Green formula, see Definition 6 and Proposition 10. It exploits a gauge freedom in Green's second identity: one can add and subtract an arbitrary boundary self-adjoint operator to the difference of the normal derivatives. This freedom can be used to get rid of the irregular part of the normal derivative and to gain regularity. In other words, the Dirichlet-to-Neumann operator is a self-adjoint operator [AM07].

The link between Grubb's and our parametrization, $(\mathcal{X}, L) \leftrightarrow U$, will be

given in Theorem 7. In a few words, the unitary U is adapted to the direct sum $H^{-1/2}(\partial\Omega) = \mathcal{X} \oplus \mathcal{X}^{\perp}$, and reads $U = V \oplus \mathbb{I}$. Here, the unitary component V is essentially the (partial) Caley transform of L and, as such, it does not have 1 as eigenvalue. Therefore, the eigenspace belonging to the eingenvalue 1 (the idle eigenspace) coincides with $\mathcal{X}^{\perp}$.
A final remark is in order. In this chapter, for definiteness, we explicitly consider only the case of the Laplace operator in a bounded regular domain of $\mathbb{R}^n$. However, Theorem 7 which establishes the link $(\mathcal{X}, L) \leftrightarrow U$, and the general strategy of encoding boundary conditions in a unitary operator by using an idle subspace and a partial Caley transform, would allow us to generalize our results to a larger class of operators (e.g. Laplace-Beltrami [ILP15c], Dirac [AIM15], pseudodifferential operators [Gru68]) and/or settings (e.g. manifolds with boundaries [ILP15a], nonregular boundaries [GM11]).
Summing up we are going to state our main result in Theorem 5. Then, after recalling Grubb's characterization of self-adjoint extensions, Theorem 6, we establish the connection betweeen the two parametrizations in Theorem 7. Then we state our result in terms of quadratic forms in Theorem 8, which is a corollary of Theorem 5. Sections 5.6 and 5.7 are devoted to the proofs of the theorems. The main properties of the Cayley transform which are used in the proofs are gathered in the final section 5.8.

5.2 Notation

We are going to consider complex separable Hilbert spaces. The inner product between two vectors u,v of a Hilbert space $\mathscr{H}$ is denoted by $\langle u|v\rangle_{\mathscr{H}}$. In our convention it is anti-linear in the first argument and linear in the second one.
Given two Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, the set of unitary operators from $\mathscr{H}_1$ to $\mathscr{H}_2$ is denoted by $\mathrm{U}(\mathscr{H}_1, \mathscr{H}_2)$, while $\mathrm{U}(\mathscr{H}_1)$ stands for $\mathrm{U}(\mathscr{H}_1, \mathscr{H}_1)$.
Let $\mathscr{H}$ be an Hilbert space and A a densely defined linear operator on $\mathscr{H}$,

$$A : D(A) \subset \mathscr{H} \to \mathscr{H}. \tag{5.1}$$

We say that A is symmetric if $\langle \psi, A\phi \rangle = \langle \phi, A\psi \rangle$ for all $\psi, \phi \in \mathscr{H}$ We are going to denote by A^* the adjoint operator of A,

$$A^* : D(A^*) \subset \mathscr{H} \quad \rightarrow \quad \mathscr{H}. \tag{5.2}$$

$$D(A^*) = \{\psi \in \mathscr{H} : \exists\, \chi \in \mathscr{H} \quad s.t. \quad \langle \psi, A\phi \rangle = \langle \chi, \phi \rangle \quad \forall \phi \in D(A)\}$$

$$\chi \ = A^*\psi \tag{5.3}$$

We say that A is *self-adjoint* if $A = A^*$. Clearly every self-adjoint operator is a symmetric operator.
We now define what we mean by an extension of a densely defined operator A. Let B a densely defined operator $B : D(B) \subset \mathscr{H} \rightarrow \mathscr{H}$, we say that B is an extension of A, if and only if $D(A) \subset D(B)$ and $A\psi = B\psi$ for all $\psi \in D(A)$.

5.3 Sobolev spaces and Trace theorems

Sobolev spaces are largely used in the mathematics community for several reasons. In particular, we will be interested in the prominent and ubiquitous role they play in boundary value problems (see section 1.1).
Let Ω be an open bounded set in $\mathbb{R}^n$, $n \in \mathbb{N}$. Let the boundary $\partial\Omega$ of Ω be a $n-1$ dimensional infinitely differentiable manifold, such that Ω is locally on one side of $\partial\Omega$. From now on a set Ω satisfying the above conditions will be called a *regular domain* [LM72]. By convention the normal ν of $\partial\Omega$ is oriented towards the exterior of Ω.
We are going to denote with $C_c^\infty(\Omega)$ the set of C^∞ functions with compact support in Ω. Moreover we are going to use the standard notation for multi-indexes, namely $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_N)$, with $\alpha_i \geq 0$ an integer and:

$$|\alpha| = \sum_{i=1}^{N} \alpha_i \qquad D^\alpha \phi = \frac{\partial^{|\alpha|}\varphi}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \ldots \partial x_N^{\alpha_N}} \tag{5.4}$$

Definition 1. Let $m \in \mathbb{N}$, $m \geq 1$, we define

$$H^m(\Omega) = \{\psi \in L^2(\Omega) \,|\, \forall \alpha \,,\, |\alpha| \leq m \,,\, D^\alpha \psi \in L^2(\Omega)\}. \tag{5.5}$$

We recall that the space H^m is a Hilbert space equipped with the scalar product:

$$\langle u, v \rangle_m = \sum_{1 \leq |\alpha| \leq m} \langle D^\alpha u, D^\alpha v \rangle, \tag{5.6}$$

where $\langle \cdot, \cdot \rangle$ in the sum in the right hand side is the scalar product in $L^2(\Omega)$.

Definition 2. We define $H_0^m(\Omega)$ as the closure in $H^m(\Omega)$ of $C_c^\infty(\Omega)$, the subspace of C^∞ functions with compact support in Ω.

More generally one can define Sobolev spaces of real order, say $H^s(\Omega)$ with $s \in \mathbb{R}$ with the usual norm [Hor63; LM72].
In the following we will be mainly interested in fractional Sobolev spaces on the border $\partial\Omega$, say $H^s(\partial\Omega)$, for which we will provide the reader with some further details.
First of all, we recall that:

Definition 3. $H^s(\mathbb{R}^n) = \{\psi \in L^2(\mathbb{R}^n) \,|\, (1 + |\xi|^2)^{s/2} \hat{\psi} \in L^2(\mathbb{R}^n)\}$, where $\hat{\psi}$ is the Fourier transform of ψ.

$H^s(\mathbb{R}^n)$ is a Hilbert space with the scalar product:

$$\langle u, v \rangle_s = \int_{\mathbb{R}^n} (1 + |\xi|^2)^s \hat{u}(\xi) \hat{v}(\xi) \mathrm{d}\xi. \tag{5.7}$$

From $\mathbb{R}^n$, then one moves on to the *half-space* $\mathbb{R}^n_+ = \{(x_1, \ldots, x_n) \,|\, x_n > 0\}$, which is the simplest prototype of an open subset with a boundary and define $H^s(\mathbb{R}^n_+)$.

Definition 4. $H^s(\mathbb{R}^n_+) = \{u \in \mathscr{D}'(\mathbb{R}^n_+) \,|\, u = U|_{\mathbb{R}^n_+} \; U \in H^s(\mathbb{R}^n)\}$, where $\mathscr{D}'(\mathbb{R}^n_+)$ is the set of distributions in $\mathbb{R}^n_+$.

Then, since every open bounded set $\Omega \subset \mathbb{R}^n$ can be locally modeled as a copy of a half-space, then, after some technical and non-trivial work one can

extend the previous results in order to define $H^s(\partial\Omega)$, $s \in \mathbb{R}$, the Sobolev space of order $s$on $\partial\Omega$ with the usual norm [Hor63; LM72].
Furthermore we set $H^s_0(\Omega)$ the closure of $C^\infty_c(\Omega)$ in $H^s(\Omega)$.
In what follows we will need the following family of operators $\{\Lambda_t\}_{t\in\mathbb{R}}$, where for all $t \in \mathbb{R}$ the operator Λ_t is defined as

$$\Lambda_t = (\mathbb{I} - \Delta_{\mathrm{LB}})^{t/2},$$

where $\mathbb{I}$ is the identity operator on $L^2(\partial\Omega)$ and Δ_{LB} is the Laplace-Beltrami operator on $\partial\Omega$. We will set $\Lambda \equiv \Lambda_1$. The family $\{\Lambda_t\}_{t\in\mathbb{R}}$ has the following property: for all $t, s \in \mathbb{R}$

$$\Lambda_t : H^s(\partial\Omega) \to H^{s-t}(\partial\Omega)$$

is positive and unitary. For an explicit construction of $\{\Lambda_t\}_{t\in\mathbb{R}}$ see [LM72].
We denote by $\langle\cdot,\cdot\rangle_{s,-s}$, with $s \in \mathbb{R}$, the pairing between $H^{-s}(\partial\Omega)$ and its dual $H^s(\partial\Omega)$ induced by the scalar product in $L^2(\partial\Omega)$, i.e.

$$\langle u, v\rangle_{s,-s} := \langle \Lambda_s u | \Lambda_{-s} v\rangle_{L^2(\partial\Omega)}, \quad \text{for all } u \in H^s(\partial\Omega), v \in H^{-s}(\partial\Omega).$$

Let H^* be the operator that acts as the distributional Laplacian on the maximal domain

$$D(H^*) = \{\psi \in L^2(\Omega) \,|\, \Delta\psi \in L^2(\Omega)\}.$$

We denote by

$$\boldsymbol{\gamma} : D(H^*) \to H^{-1/2}(\partial\Omega), \quad \psi \mapsto \boldsymbol{\gamma}(\psi) = \psi|_{\partial\Omega}$$

the *trace operator*, and by

$$\boldsymbol{\nu} : D(H^*) \to H^{-3/2}(\partial\Omega), \quad \psi \mapsto \boldsymbol{\nu}(\psi) = \frac{\partial\psi}{\partial\nu} = (\nabla\psi)|_{\partial\Omega} \cdot \nu$$

the *normal derivative*, and we recall that these operators are continuous with respect to the graph norm of H^* [LM72].

In the following we will consider the Laplace operator $H = -\Delta$ on the domain

$$D(H) = \{\psi \in H^2(\Omega) \,|\, \boldsymbol{\gamma}\psi = \boldsymbol{\nu}\psi = 0\} \equiv H_0^2(\Omega), \tag{5.8}$$

and the Dirichlet Laplacian, $H_{\mathrm{D}} = -\Delta$ on

$$D(H_{\mathrm{D}}) = H^2(\Omega) \cap H_0^1(\Omega) = \{\psi \in H^2(\Omega) \,|\, \boldsymbol{\gamma}\psi = 0\}. \tag{5.9}$$

We recall that H is nothing but the closure in $L^2(\Omega)$ of the symmetric operator given by the Laplacian on functions in $C_c^\infty(\Omega)$. Moreover, H_{D} is a self-adjoint, positive-definite operator, $H_{\mathrm{D}} = H_{\mathrm{D}}^* > 0$.
Moreover H^* is the adjoint operator of the symmetric operator H, and H_{D} is a self-adjoint extension of H, namely,

$$H \subset H_{\mathrm{D}} \subset H^*.$$

Our main objective is to characterize all the possible self-adjoint extensions of the symmetric operator H. As the Dirichlet Laplacian, they will all be contained between the minimal Laplacian H and the maximal one H^*. The domain of each self-adjoint extension will be characterized by a specific relation between the values of the functions and those of their normal derivatives at the boundary.
As already discussed in section 1.6 in quantum mechanics every self-adjoint extension represents the kinetic energy operator of a free nonrelativistic particle (with $\hbar^2/2m = 1$), constrained in the spatial domain Ω by a suitable specific wall.
We will need a regularized version of the trace operator for the normal derivative $\boldsymbol{\nu}$.

Definition 5. The *regularized normal derivative* $\boldsymbol{\mu} : D(H^*) \to H^{-1/2}(\partial\Omega)$ is the linear operator whose action is

$$\boldsymbol{\mu}\psi = \Lambda\, \boldsymbol{\nu}\Pi_{\mathrm{D}}\psi,$$

for all $\psi \in D(H^*)$, where $\Pi_{\mathrm{D}} = H_{\mathrm{D}}^{-1}H^*$.

Remark 1. Note that H_{D}^{-1} maps $L^2(\Omega)$ onto $D(H_{\mathrm{D}}) \subset H^2(\Omega)$. By the trace theorem, $\boldsymbol{\nu}(H^2(\Omega)) = H^{1/2}(\partial\Omega)$, whence $\boldsymbol{\mu}\psi \in H^{-1/2}(\partial\Omega)$ is more regular than the normal derivative $\boldsymbol{\nu}\psi \in H^{-3/2}(\partial\Omega)$.
The operator Π_{D} is in fact a (nonorthogonal) projection from $D(H^*)$ onto $D(H_{\mathrm{D}})$, since for all $\psi \in D(H_{\mathrm{D}})$ one gets that $\Pi_{\mathrm{D}}\psi = H_{\mathrm{D}}^{-1}H^*\psi = H_{\mathrm{D}}^{-1}H_{\mathrm{D}}\psi = \psi$. Thus, $\boldsymbol{\mu}\psi$ is the image under Λ of the normal derivative of the component $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi$ of ψ belonging to the regular subspace $D(H_{\mathrm{D}})$ of $D(H^*)$.

5.4 The theorems

In this section we are going to briefly state, without proof, the theorems which mainly characterize the mutual relation between the self-adjoint extensions of the Hamiltonian H and the boundary conditions on Ω. In particular in Theorem 5 every self-adjoint extension of H is parametrized in terms of a unitary operator U in $\mathrm{U}(H^{-1/2}(\partial\Omega))$:

Theorem 5. *The set of all self-adjoint extensions of H is*

$$\left\{H_U : D(H_U) \to L^2(\Omega) \,|\, U \in \mathrm{U}(H^{-1/2}(\partial\Omega))\right\},$$

where for all $U \in \mathrm{U}(H^{-1/2}(\partial\Omega))$

$$D(H_U) = \{\psi \in D(H^*) \,|\, i(\mathbb{I} + U)\boldsymbol{\gamma}\psi = (\mathbb{I} - U)\boldsymbol{\mu}\psi\}.$$

Remark 2. It is interesting to stress the role played by the regularized normal derivative $\boldsymbol{\mu}\psi$ in the above theorem: the trace $\boldsymbol{\gamma}\psi$ and $\boldsymbol{\mu}\psi$ can be compared because they both belong to the same (boundary) space, namely $H^{-1/2}(\partial\Omega)$. Notice also the equivalent relation

$$\boldsymbol{\mu}\psi - i\boldsymbol{\gamma}\psi = U(\boldsymbol{\mu}\psi + i\boldsymbol{\gamma}\psi)$$

defining the domain of the self adjoint extension H_U.

Next we want to compare the result in Theorem 5 with the classical characterization of the self-adjoint extensions of H due to Grubb [Gru09; Gru68].

We need some notation: a closed linear subspace $\mathcal{X}$ of $H^{-1/2}(\partial\Omega)$ is denoted by $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$, and $\mathcal{X}^*$ denotes its dual; we say that a densely defined operator $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ is self-adjoint if

$$\Lambda L : D(L) \subset \mathcal{X} \to \mathcal{X}$$

is self-adjoint, $(\Lambda L)^* = \Lambda L$.

Theorem 6 ([Gru68])**.** *The set of all self-adjoint extensions of H is*

$$\left\{ H_{(\mathcal{X},L)} : D\left(H_{(\mathcal{X},L)}\right) \to L^2(\Omega) \right\},$$

that is to say:

$$\left\{ H_{(\mathcal{X},L)} \,|\, \mathcal{X} \sqsubset H^{-1/2}(\partial\Omega),\ L : D(L) \subset \mathcal{X} \to \mathcal{X}^*, L \text{ self-adjoint} \right\},$$

where, for all $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ and $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$, L self-adjoint,

$$D\left(H_{(\mathcal{X},L)}\right) =$$
$$= \{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in D(L),\ \langle \boldsymbol{\nu}\Pi_{\mathrm{D}}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}} = \langle L\boldsymbol{\gamma}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}},\ \forall u \in \mathcal{X}\}.$$

The relation between the two different parametrizations of the self-adjoint extensions of H given in Theorem 5 and Theorem 6 is established in the next theorem. First we introduce some notation: if $U : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ is a linear operator and $\mathcal{X}$ is a subspace of $H^{-1/2}(\partial\Omega)$ we denote by $U\restriction_{\mathcal{X}}$ the operator

$$U\restriction_{\mathcal{X}}\colon \mathcal{X} \to U(\mathcal{X}), \qquad u \in \mathcal{X} \mapsto Uu.$$

Then the relation between the two different parametrization is given by:

Theorem 7. *For all $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ and $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$, with L self-adjoint, it results that*

$$H_{(\mathcal{X},L)} = H_U, \quad \textit{with } U = \mathscr{C}(\Lambda L) \oplus \mathbb{I}_{\mathcal{X}^\perp} \in \mathrm{U}(H^{-1/2}(\partial\Omega)),$$

where

$$\mathscr{C}(\Lambda L) = (\Lambda L - i\mathbb{I}_{\mathcal{X}})(\Lambda L + i\mathbb{I}_{\mathcal{X}})^{-1}$$

is the Cayley transform of ΛL*, and* $\mathbb{I}_{\mathcal{X}}, \mathbb{I}_{\mathcal{X}^\perp}$ *are the identity operators on* $\mathcal{X}$ *and on* $\mathcal{X}^\perp$*, respectively.*
Conversely for all $U \in \mathrm{U}(H^{-1/2}(\partial\Omega))$ *it results that*

$$H_U = H_{(\mathcal{X},L)}, \text{ with } \mathcal{X} = \operatorname{Ran} Q_U \text{ and } L = \Lambda^{-1}\mathscr{C}^{-1}\left(U\restriction_{\mathcal{X}}\right),$$

where Q_U *is the spectral projection of* U *on the Borel set* $\mathbb{R} \setminus \{1\}$ *and*

$$\mathscr{C}^{-1}(V) = i\left(\mathbb{I}_{\mathcal{X}} + V\right)\left(\mathbb{I}_{\mathcal{X}} - V\right)^{-1}$$

is the inverse Cayley transform of $V \in \mathrm{U}(\mathcal{X})$*.*

Remark 3. The Cayley transform maps bijectively self-adjoint operators on the Hilbert space $\mathcal{X}$ to unitary operators that do not have 1 as eigenvalue. See Section 5.8. In the second part of the theorem, $V = U\restriction_{\mathcal{X}}$ is the restriction of the unitary U to its spectral subspace $\mathcal{X} = \operatorname{Ran} Q_U$ orthogonal to the (possible) eigenspace belonging to the eigenvalue 1. Therefore its inverse Cayley transform exists. It is a bounded self-adjoint operator if 1 is a point of the resolvent set of V, i.e. if the (possible) eigenvalue 1 of U is isolated; otherwise it is an unbounded self-adjoint operator.

5.5 Quadratic forms and expectation values

In this section we are going to discuss and prove a representation theorem for the self-adjoint extensions of the observable H in terms of energy expectation values.
Consider the expectation value of the symmetric operator $H = -\Delta$ at $\psi \in D(H) = H_0^2(\Omega)$:

$$\mathfrak{t}(\psi) = \langle\psi|H\psi\rangle_{L^2(\Omega)} = \|\nabla\psi\|^2_{L^2(\Omega)}. \tag{5.10}$$

Physically this represents the kinetic energy of a quantum particle in the vector state ψ (assumed to be normalized). According to the postulates of

quantum mechanics, a quadratic form corresponds to a physical observable—and hence to a self-adjoint operator—if and only if it is real and closed [RS75]. Therefore, the search of the self-adjoint extensions of the symmetric operator H is mirrored in the search of the real and closed quadratic forms that extend the minimal form (5.10).
As a consequence, Theorem 5 has a counterpart in terms of kinetic energy forms, through the relation $\mathfrak{t}_U(\psi) = \langle\psi|H_U\psi\rangle$, which must hold for all $\psi \in D(H_U)$.

Theorem 8. *The set of all real closed quadratic forms on $L^2(\Omega)$ that extend $\mathfrak{t}(\psi)$ is*

$$\left\{\mathfrak{t}_U : D(\mathfrak{t}_U) \to \mathbb{R} \,|\, U \in \mathrm{U}(H^{-1/2}(\partial\Omega))\right\},$$

with

$$\mathfrak{t}_U(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\boldsymbol{\gamma}\psi|K_U\boldsymbol{\gamma}\psi\rangle_{H^{-1/2}(\partial\Omega)}, \qquad \textit{for all } \psi \in D_U,$$

where

$$D_U = D(\mathfrak{t}_{\mathrm{D}}) + N(H^*) \cap \boldsymbol{\gamma}^{-1}\left(D(K_U)\right)$$

is a core of $\mathfrak{t}_U$.
Here $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi \in D(\mathfrak{t}_{\mathrm{D}}) = H^1_0(\Omega)$, the domain of the Dirichlet form, and K_U is a self-adjoint operator on the boundary space $H^{-1/2}(\partial\Omega)$ defined by

$$D(K_U) = \mathrm{Ran}(\mathbb{I} - U),$$

$$K_U(\mathbb{I} - U)g = -iQ_U(\mathbb{I} + U)g, \qquad \textit{for all } g \in H^{-1/2}(\partial\Omega),$$

with Q_U the projection onto the subspace $\overline{\mathrm{Ran}(\mathbb{I} - U)}$.
Moreover, the domain $D(H_U)$ of Theorem 5 is a core of $\mathfrak{t}_U$ (in fact it is a subspace of D_U), and

$$\mathfrak{t}_U(\psi) = \langle\psi|H_U\psi\rangle_{L^2(\Omega)} \qquad \textit{for all } \psi \in D(H_U).$$

Proof. According to assertion 2 of Lemma 9, every $\phi \in C^\infty(\overline{\Omega}) \subset D(H^*)$ has a unique decomposition $\phi = \phi_{\mathrm{D}} + \phi_0$, with $\boldsymbol{\gamma}\phi_{\mathrm{D}} = 0$ and $\Delta\phi_0 = 0$. Thus, for

any $\phi \in C^\infty(\overline{\Omega})$, we get by the Gauss-Green formula and Definition 5

$$\begin{aligned}\langle\phi|H^*\phi\rangle_{L^2(\Omega)} &= -\int_\Omega \bar{\phi}\Delta\phi_{\mathrm{D}}\mathrm{d}x \\ &= \int_\Omega \nabla\bar{\phi}_0\cdot\nabla\phi_{\mathrm{D}}\mathrm{d}x + \int_\Omega |\nabla\phi_{\mathrm{D}}|^2\mathrm{d}x - \int_{\partial\Omega}\bar{\phi}\frac{\partial\phi_{\mathrm{D}}}{\partial\nu}\mathrm{d}S \\ &= \|\nabla\phi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle\boldsymbol{\gamma}\phi|\boldsymbol{\mu}\phi\rangle_{H^{-1/2}(\partial\Omega)}, \end{aligned} \tag{5.11}$$

since

$$\int_\Omega \nabla\bar{\phi}_0\cdot\nabla\phi_{\mathrm{D}}\mathrm{d}x = -\int_\Omega \Delta\bar{\phi}_0\phi_{\mathrm{D}}\mathrm{d}x + \int_{\partial\Omega}\frac{\partial\bar{\phi}_0}{\partial\nu}\phi_{\mathrm{D}}\mathrm{d}S = 0.$$

By density, formula (5.11) is valid for all $\phi \in D(H^*)$. Therefore, we can define the following quadratic form

$$\mathfrak{t}_*(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle\boldsymbol{\gamma}\psi|\boldsymbol{\mu}\psi\rangle_{H^{-1/2}(\partial\Omega)}, \tag{5.12}$$

which on $D(H^*)$ coincides with the expectation value of the operator H^*, namely

$$\mathfrak{t}_*(\psi) = \langle\psi|H^*\psi\rangle_{L^2(\Omega)},$$

for all $\psi \in D(H^*)$. However, notice that $D(H_{\mathrm{D}}) = H^2(\Omega)\cap H^1_0(\Omega)$ is a dense subspace of $D(\mathfrak{t}_{\mathrm{D}}) = H^1_0(\Omega)$, the domain of the Dirichlet quadratic form,

$$\mathfrak{t}_{\mathrm{D}}(u) = \|\nabla u\|^2_{L^2(\Omega)}.$$

Therefore, the form (5.12) can be extended by density to functions

$$\psi \in D(\mathfrak{t}_{\mathrm{D}}) + N(H^*).$$

[Recall the decomposition of Lemma 9, $D(H^*) = D(H_{\mathrm{D}}) + N(H^*)$.]
Suppose now that $\psi \in D(H_U) \subset D(H^*)$. Thus,

$$\langle\psi|H_U\psi\rangle_{L^2(\Omega)} = \mathfrak{t}_*(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle\boldsymbol{\gamma}\psi|\boldsymbol{\mu}\psi\rangle_{H^{-1/2}(\partial\Omega)},$$

and, by Theorem 5,

$$i(\mathbb{I}+U)\boldsymbol{\gamma}\psi = (\mathbb{I}-U)\boldsymbol{\mu}\psi.$$

Let P_U and Q_U be the spectral projections of U on the Borel sets $\{1\}$ and $\mathbb{R} \setminus \{1\}$, respectively ($P_U$ is zero if 1 is not an eigenvalue of U). Then the above relation is equivalent to

$$P_U \boldsymbol{\gamma}\psi = 0, \qquad i(\mathbb{I}+U)Q_U\boldsymbol{\gamma}\psi = (\mathbb{I}-U)Q_U\boldsymbol{\mu}\psi, \tag{5.13}$$

which imply that

$$\boldsymbol{\gamma}\psi \in \operatorname{Ran}(\mathbb{I}-U) \subset \operatorname{Ran} Q_U,$$

since $\operatorname{Ran} P_U = \operatorname{Ran}(\mathbb{I}-U)^{\perp}$. Let us now define the operator K_U with domain

$$D(K_U) = \operatorname{Ran}(\mathbb{I}-U),$$

whose action is

$$K_U(\mathbb{I}-U)g = -iQ_U(\mathbb{I}+U)g = -i(\mathbb{I}+U)Q_U g,$$

for all $g \in H^{-1/2}(\partial\Omega)$. Thus we get that, for some $g \in H^{-1/2}(\partial\Omega)$,

$$\begin{aligned} i(\mathbb{I}+U)Q_U\boldsymbol{\gamma}\psi &= i(\mathbb{I}+U)Q_U(\mathbb{I}-U)g = (\mathbb{I}-U)iQ_U(\mathbb{I}+U)g \\ &= -(\mathbb{I}-U)K_U(\mathbb{I}-U)g = -(\mathbb{I}-U)K_UQ_U\boldsymbol{\gamma}\psi, \end{aligned}$$

which plugged into (5.13) gives

$$-(\mathbb{I}-U)Q_UK_U\boldsymbol{\gamma}\psi = (\mathbb{I}-U)Q_U\boldsymbol{\mu}\psi.$$

Since $\mathbb{I}-U$ is injective when restricted to $\operatorname{Ran} Q_U$, we get that

$$K_U\boldsymbol{\gamma}\psi = -Q_U\boldsymbol{\mu}\psi, \tag{5.14}$$

for all $\boldsymbol{\gamma}\psi \in D(K_U)$. This implies that

$$-\langle \boldsymbol{\gamma}\psi | \boldsymbol{\mu}\psi \rangle_{H^{-1/2}(\partial\Omega)} = \langle \boldsymbol{\gamma}\psi | K_U\boldsymbol{\gamma}\psi \rangle_{H^{-1/2}(\partial\Omega)},$$

for all $\psi \in D(\mathfrak{t}_{\mathrm{D}}) + N(H^*)$, such that $\boldsymbol{\gamma}\psi \in D(K_U)$.

Thus we can define the quadratic form

$$\mathfrak{t}_U(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle\boldsymbol{\gamma}\psi|K_U\boldsymbol{\gamma}\psi\rangle_{H^{-1/2}(\partial\Omega)},$$

on the domain

$$D_U = D(\mathfrak{t}_{\mathrm{D}}) + N(H^*) \cap \boldsymbol{\gamma}^{-1}\left(D(K_U)\right).$$

For all $\psi \in D(H_U)$ it coincides with the expectation value of the self-adjoint extension H_U:

$$\mathfrak{t}_U(\psi) = \langle\psi|H_U\psi\rangle_{L^2(\Omega)}.$$

The domain D_U is a core of the quadratic form $\mathfrak{t}_U$ since it contains the domain of its associated self-adjoint operator H_U, namely $D(H_U) \subset D_U$. □

Remark 4. At variance with the domains of their corresponding operators, the domains of the kinetic energy forms are all contained between a minimal domain and a maximal one:

$$D(\mathfrak{t}_{\mathbb{I}}) \subset D(\mathfrak{t}_U) \subset D(\mathfrak{t}_{-\mathbb{I}}).$$

The Dirichlet form $\mathfrak{t}_{\mathbb{I}} = \mathfrak{t}_{\mathrm{D}}$ has the expression

$$\mathfrak{t}_{\mathrm{D}}(\psi) = \|\nabla\psi\|^2_{L^2(\Omega)},$$

on the minimal domain $D(\mathfrak{t}_{\mathrm{D}}) = H^1_0(\Omega)$, while the form $\mathfrak{t}_{-\mathbb{I}}$ has maximal domain $D(\mathfrak{t}_{-\mathbb{I}}) = H^1_0(\Omega) + N(H^*)$ and acts as

$$\mathfrak{t}_{-\mathbb{I}}(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)}.$$

Both forms have no boundary term, since the boundary Hamiltonians are both zero, $K_{\mathbb{I}} = K_{-\mathbb{I}} = 0$, but on the smallest and largest domain, respectively: $D(K_{\mathbb{I}}) = \{0\}$ and $D(K_{-\mathbb{I}}) = H^{-1/2}(\partial\Omega)$. The maximal form $\mathfrak{t}_{-\mathbb{I}}$ corresponds to the Kreĭn-von Neumann extension $H_{-\mathbb{I}}$, whose boundary condition is the vanishing of the regularized normal derivative, $\boldsymbol{\mu}\psi = 0$ [Kre47].

Remark 5. Notice that the boundary Hamiltonian K_U is nothing but the

inverse partial Cayley transform of the unitary U on its spectral subspace $\mathrm{Ran}\, Q_U = \overline{\mathrm{Ran}\,(\mathbb{I} - U)}$. (In the above proof Q_U has been identified as the spectral projection of U on the Borel set $\mathbb{R} \setminus \{1\}$). Explicitly, one gets

$$K_U = -\mathscr{C}^{-1}(U\restriction_{\mathrm{Ran}\, Q_U}).$$

The inverse Cayley transform is well defined since the restriction of U has the eigenvalue 1 stripped out. Notice, however, that if 1 is not an isolated eigenvalue of U, then 1 is not in the resolvent set of $U\restriction_{\mathrm{Ran}\, Q_U}$, and thus K_U is an unbounded operator.

Remark 6. Theorem 6 estabilishes a one-to-one correspondence between the set of the self-adjoint extensions of H and the set of pairs $(\mathcal{X}, L)$ composed of a closed subspace $\mathcal{X}$ and a self-adjoint operator L.
In addition to that, it was proved in [Gru74] that a self-adjoint extension of H is bounded from below if and only if the operator L is bounded from below. Something more can be said in terms of the parametrization with unitary operators. Indeed, since $K_U = -\mathscr{C}^{-1}(U\restriction_{\mathrm{Ran}\, Q_U})$, and $U\restriction_{\mathrm{Ran}\, Q_U} = \mathscr{C}(\Lambda L)$, it follows that a self-adjoint extension of H is bounded from below if and only if the corresponding operator K_U is bounded from below.
The above statement can be rephrased in terms of U. In particular if K_U is bounded, then, there is a whole gap around the point $(x, y) = (1, 0)$ on the unit circle, where the spectrum of U is settled.
Instead, K_U is bounded from below if and only the spectrum of U has a gap just below the point $(1, 0)$. Namely the set $\{\mathrm{e}^{\mathrm{i}\alpha} : \alpha \in (-\varepsilon, 0)\}$ belongs to the resolvent set of U for some $\varepsilon > 0$.
Summing up, if $1 \in \rho(U\restriction_{\mathrm{Ran}\, Q_U})$, then for sure K_U is a bounded operator. Instead, if there is a semi-gap from below around the point $(1, 0)$, then K_U is solely bounded from below.

5.6 Theorem 5: the proof

In this section we are going to explicitly prove the characterization theorem of the self-adjoint extensions of H in terms of unitary operators.

We will first need some properties of the regularized normal derivative μ and of the projection Π_{D}.

Lemma 9. *The following properties hold:*

1. *Let $\boldsymbol{\mu}$ be the regularized normal derivative of Definition 5, then*

$$\boldsymbol{\mu} : D(H^*) \to H^{-1/2}(\partial\Omega)$$

is a surjective continuous map with respect to the graph norm.

2. *The domain of the adjoint $D(H^*)$ is the vector space direct sum of the domain of the Dirichlet Laplacian H_{D} and the kernel of H^*:*

$$D(H^*) = D(H_{\mathrm{D}}) + N(H^*), \qquad \psi = \psi_{\mathrm{D}} + \psi_0,$$

where $\psi \in D(H^*)$, $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi \in D(H_{\mathrm{D}})$, and $\psi_0 = (\mathbb{I} - \Pi_{\mathrm{D}})\psi \in N(H^*)$.

3. *The map*

$$\phi \in D(H^*) \mapsto (\boldsymbol{\gamma}\,\phi, \boldsymbol{\mu}\,\phi) \in H^{-1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$$

is surjective.

Proof. 1. The map $\boldsymbol{\mu}$ is continuous as a composition of three continuous maps: $\boldsymbol{\mu} = \Lambda\boldsymbol{\nu}\Pi_{\mathrm{D}}$, with $\Lambda : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ being unitary,

$$\boldsymbol{\nu} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$$

being continuous by the trace theorem, and

$$\Pi_{\mathrm{D}} = H_{\mathrm{D}}^{-1} H^* : D(H^*) \to D(H_{\mathrm{D}}) = H^2(\Omega) \cap H_0^1(\Omega)$$

being a projection, as pointed out in Remark 1.

Surjectivity follows from the surjectivity of the projection Π_{D} and from the surjectivity of the map

$$\boldsymbol{\gamma}_1 = (\boldsymbol{\gamma}, \boldsymbol{\nu}) : H^2(\Omega) \to H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega),$$

which implies the surjectivity of its restriction

$$\boldsymbol{\gamma}_1 : H^2(\Omega) \cap \boldsymbol{\gamma}_1^{-1}(\{0\} \times H^{1/2}(\partial\Omega)) \to \{0\} \times H^{1/2}(\partial\Omega),$$

and thus of the map

$$\boldsymbol{\nu} : H^2(\Omega) \cap H_0^1(\Omega) \to H^{1/2}(\partial\Omega).$$

2. For any $\psi \in D(H^*)$ we have $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi \in D(H_{\mathrm{D}})$ and $\psi_0 = (\mathbb{I} - \Pi_{\mathrm{D}})\psi \in N(H^*)$. Indeed,

$$H^*\psi_0 = H^*\psi - H^*\Pi_{\mathrm{D}}\psi = H^*\psi - H^*H_{\mathrm{D}}^{-1}H^*\psi = H^*\psi - H_{\mathrm{D}}H_{\mathrm{D}}^{-1}H^*\psi = 0.$$

3. Since $\Lambda : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ is unitary, the surjectivity of the map

$$(\boldsymbol{\gamma}, \boldsymbol{\mu}) : D(H^*) \to H^{-1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$$

is equivalent to the surjectivity of

$$(\boldsymbol{\gamma}, \boldsymbol{\nu}\Pi_{\mathrm{D}}) : D(H^*) \to H^{-1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega).$$

By the decomposition of point 2 of the Lemma, we get that for any $\psi \in D(H^*)$, $\psi = \psi_{\mathrm{D}} + \psi_0$ with $\boldsymbol{\gamma}\psi_{\mathrm{D}} = 0$ and $\boldsymbol{\nu}\Pi_{\mathrm{D}}\psi_0 = \boldsymbol{\nu}\Pi_{\mathrm{D}}(\mathbb{I} - \Pi_{\mathrm{D}})\psi = 0$. Therefore,

$$(\boldsymbol{\gamma}, \boldsymbol{\nu}\Pi_{\mathrm{D}})\psi = (\boldsymbol{\gamma}\psi_0, \boldsymbol{\nu}\psi_{\mathrm{D}}).$$

Therefore, the surjectivity of $(\boldsymbol{\gamma}, \boldsymbol{\mu})$ follows from the separate surjectivity of the two component maps:

$$\boldsymbol{\gamma} : N(H^*) \to H^{-1/2}(\partial\Omega), \qquad \boldsymbol{\nu} : D(H_{\mathrm{D}}) \to H^{1/2}(\partial\Omega).$$

The surjectivity of $\boldsymbol{\nu}$ has just been proved in part 1. The surjectivity of $\boldsymbol{\gamma}$ is nothing but a classical result [Tre06] on the existence of an $L^2(\Omega)$-solution to the Laplace equation $-\Delta u = 0$ for any Dirichlet boundary condition $\boldsymbol{\gamma}u = g \in H^{-1/2}(\partial\Omega)$.

□

Using the regularity result in Lemma 9 we can define the generalized Gauss-Green boundary form.

Definition 6. We define the generalized Gauss-Green boundary form

$$\Gamma : D(H^*) \times D(H^*) \to \mathbb{C}$$

such that for all $\phi, \psi \in D(H^*)$

$$\Gamma(\phi, \psi) = \langle \boldsymbol{\mu}\phi | \boldsymbol{\gamma}\psi \rangle_{H^{-1/2}(\partial\Omega)} - \langle \boldsymbol{\gamma}\phi | \boldsymbol{\mu}\psi \rangle_{H^{-1/2}(\partial\Omega)}.$$

In [Gru68] it was proved the following result:

Proposition 10. *Let H the operator defined in (5.8) and let Γ the generalized Gauss-Green boundary form in Definition 6. Then*

$$\Gamma(\phi, \psi) = \langle \phi | H^*\psi \rangle_{L^2(\Omega)} - \langle H^*\phi | \psi \rangle_{L^2(\Omega)} \quad \textit{for all } \phi, \psi \in D(H^*). \tag{5.15}$$

Proof. According to Lemma 9.2, every $\phi \in C^\infty(\overline{\Omega}) \subset D(H^*)$ has a unique decomposition $\phi = \phi_{\mathrm{D}} + \phi_0$, with $\boldsymbol{\gamma}\phi_{\mathrm{D}} = 0$ and $\Delta\phi_0 = 0$. Thus, for any $\phi, \psi \in C^\infty(\overline{\Omega})$, we get

$$\begin{aligned}
&\langle \phi | H^*\psi \rangle_{L^2(\Omega)} - \langle H^*\phi | \psi \rangle_{L^2(\Omega)} = \int_\Omega \left(\Delta\bar{\phi}_{\mathrm{D}}\psi - \bar{\phi}\Delta\psi_{\mathrm{D}} \right) \mathrm{d}x \\
&= \int_{\partial\Omega} \left(\frac{\partial\bar{\phi}_{\mathrm{D}}}{\partial\nu}\psi - \bar{\phi}\frac{\partial\psi_{\mathrm{D}}}{\partial\nu} \right) \mathrm{d}S = \langle \boldsymbol{\nu}\phi_{\mathrm{D}}, \boldsymbol{\gamma}\psi \rangle_{\frac{1}{2},-\frac{1}{2}} - \langle \boldsymbol{\gamma}\phi, \boldsymbol{\nu}\psi_{\mathrm{D}} \rangle_{-\frac{1}{2},\frac{1}{2}} \\
&= \langle \boldsymbol{\mu}\phi | \boldsymbol{\gamma}\psi \rangle_{H^{-1/2}(\partial\Omega)} - \langle \boldsymbol{\gamma}\phi | \boldsymbol{\mu}\psi \rangle_{H^{-1/2}(\partial\Omega)},
\end{aligned}$$

by the Gauss-Green formula and Definition 5. The result follows by density.

□

We denote by $\mathscr{H}_b := H^{-1/2}(\partial\Omega) \oplus H^{-1/2}(\partial\Omega)$.

Definition 7. Let $\mathcal{W}$ be a subspace of $\mathscr{H}_{\mathrm{b}}$. We define the Γ-*orthogonal* subspace of $\mathcal{W}$ as

$$\mathcal{W}^\dagger := \left\{ (u_1, u_2) \in \mathscr{H}_{\mathrm{b}} \,\middle|\, \langle u_2 | v_1 \rangle_{H^{-1/2}(\partial\Omega)} = \langle u_1 | v_2 \rangle_{H^{-1/2}(\partial\Omega)},\ \forall (v_1, v_2) \in \mathcal{W} \right\}.$$

We say that $\mathcal{W}$ is a *maximally isotropic* subspace if $\mathcal{W} = \mathcal{W}^\dagger$.

Proposition 11. *Let $\mathcal{W}$ be a subspace of $\mathscr{H}_b$ and let $\tilde{H}$ be the restriction of H^* to the domain*

$$D(\tilde{H}) = \{\phi \in D(H^*) \,|\, (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W}\}\,.$$

Then $\tilde{H}$ is self-adjoint if and only if $\mathcal{W}$ is a closed maximally isotropic subspace.

Proof. First of all we observe that

$$\tilde{H} \text{ is self-adjoint } \iff \mathcal{G}(\tilde{H}^*) = \mathcal{G}(\tilde{H})$$

and that $D(\tilde{H}) \subset D(\tilde{H}^*) \subset D(H^*)$. The proof follows immediately by observing that the graph of $\tilde{H}$ reads

$$\begin{aligned}\mathcal{G}(\tilde{H}) &= \left\{(\phi, H^*\phi) \,\middle|\, \phi \in D(\tilde{H})\right\} \\ &= \left\{(\phi, H^*\phi) \,\middle|\, \phi \in D(H^*),\ (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W}\right\},\end{aligned}$$

while the graph of $\tilde{H}^*$ is

$$\begin{aligned}\mathcal{G}(\tilde{H}^*) &= \left\{(\phi, H^*\phi) \,\middle|\, \phi \in D(\tilde{H}^*)\right\} \\ &= \left\{(\phi, H^*\phi) \,\middle|\, \phi \in D(H^*),\ \Gamma(\phi, \psi) = 0,\ \forall \psi \in D(\tilde{H})\right\}\end{aligned}$$

Using the definition of Γ, $\mathcal{G}(\tilde{H}^*)$ reads:

$$\left\{(\phi, H^*\phi) \,|\, \phi \in D(H^*), \langle u_1 | \boldsymbol{\mu}\phi\rangle_{H^{-1/2}(\partial\Omega)} = \langle \boldsymbol{\gamma}\phi | u_2\rangle_{H^{-1/2}(\partial\Omega)}, \forall (u_1, u_2) \in \mathcal{W}\right\},$$

that is:

$$\mathcal{G}(\tilde{H}^*) = \left\{(\phi, H^*\phi) \,|\, \phi \in D(H^*),\ (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W}^\dagger\right\},$$

and thus $\mathcal{G}(\tilde{H}) = \mathcal{G}(\tilde{H}^*)$ iff $\mathcal{W} = \mathcal{W}^\dagger$. □

The closed maximally isotropic subspaces are characterized by the following theorem, whose straightforward proof can be found in [BGP08].

Theorem 12. *A closed subspace $\mathcal{W}$ of $\mathscr{H}_b$ is a maximally isotropic subspace if and only if there exists $U \in \mathrm{U}(H^{-1/2}(\partial\Omega))$ such that*

$$\mathcal{W} = \{(u_1, u_2) \in \mathscr{H}_b \,|\, i(\mathbb{I} + U)u_1 = (\mathbb{I} - U)u_2\}\,.$$

We can now conclude.

Proof of Theorem 5. The proof follows immediately from Proposition 11 and Theorem 12. □

Remark 7. The proof of Theorem 5 can be translated into the language of boundary triples [BGP08], by saying that $(\mathscr{H}_{\mathrm{b}}, \boldsymbol{\gamma}, \boldsymbol{\mu})$ is a boundary triple for H^*. This follows by Proposition 10 and by assertion 3 of Lemma 9.

5.7 Theorem 7: the proof

In this section we are going to prove Theorem 7, which links the parametrization of self-adjoint extensions of H given by Grubb, with the one provided in Theorem 5.

Proof. Let $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ and $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ a self-adjoint operator. For all $\psi \in D(T^*)$ we denote by $(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}$ the element of $\mathcal{X}^*$ defined as follows:

$$(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} u := \langle \Lambda_{-1}\boldsymbol{\mu}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}}, \qquad \text{for all } u \in \mathcal{X},$$

thus we have that

$$D(H_{(\mathcal{X},L)}) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in D(L),\, (\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} = L\boldsymbol{\gamma}\psi\right\}.$$

The operator $\Lambda L : D(\Lambda L) \subset \mathcal{X} \to \mathcal{X}$ is self-adjoint, where $D(\Lambda L) = D(L)$. We can define

$$V = \mathscr{C}(\Lambda L) = (\Lambda L - i\mathbb{I}_{\mathcal{X}})(\Lambda L + i\mathbb{I}_{\mathcal{X}})^{-1}$$

and by Proposition 13 in Section 5.8 we have that $V \in \mathrm{U}(\mathcal{X})$. Now observe

that, by assertion 4 of Proposition 13, we can rewrite $D(H_{(\mathcal{X},L)})$ as follows

$$D(H_{(\mathcal{X},L)}) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in D(\Lambda L),\, i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}.$$

For all $\psi \in D(H^*)$ we denote by $(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}$ the element of $\mathcal{X}$ defined as follows:

$$v(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} := \langle v, \boldsymbol{\mu}\psi\rangle_{\frac{1}{2},-\frac{1}{2}}, \qquad \text{for all } v \in \mathcal{X}^*,$$

Observe that

$$\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} = (\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} \quad \text{for all } \psi \in D(H^*),$$

therefore $D(H_{(\mathcal{X},L)})$ can be rewritten as

$$D(H_{(\mathcal{X},L)}) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in D(\Lambda L),\, i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

By Lemma 14 in Sec. 5.8, one gets that the condition $\boldsymbol{\gamma}\psi \in D(\Lambda L)$ can be dispensed with. Indeed, as long as $\boldsymbol{\gamma}\psi \in \mathcal{X}$ satisfies the equation

$$i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}},$$

then $\boldsymbol{\gamma}\psi \in D(\Lambda L)$. Therefore we have proved that

$$D(H_{(\mathcal{X},L)}) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in \mathcal{X},\, i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

Thus, by defining the operator $U := V \oplus \mathbb{I}_{\mathcal{X}^\perp} \in \mathrm{U}(H^{-1/2}(\partial\Omega))$, we have that $D(H_{(\mathcal{X},L)}) = D(H_U)$, and that $H_{(\mathcal{X},L)} = H_U$ with $U := \mathscr{C}(\Lambda L) \oplus \mathbb{I}_{\mathcal{X}^\perp}$.
Now we prove the converse. Fix $U \in \mathrm{U}(H^{-1/2}(\partial\Omega))$ and consider H_U, a self-adjoint extension of H. Let P_U the spectral projection of U on the Borel set $\{1\} \subset \mathbb{R}$. Define $\mathcal{X} := \mathrm{Ran}(P_U)^\perp \sqsubset H^{-1/2}(\partial\Omega)$ and consider the operator $V = U\restriction_{\mathcal{X}} \in \mathrm{U}(\mathcal{X})$. Clearly, 1 is not an eigenvalue of V, therefore we can define the self-adjoint operator

$$L := \Lambda^{-1}\left[i(\mathbb{I}_{\mathcal{X}} + V)(\mathbb{I}_{\mathcal{X}} - V)^{-1}\right] : D(L) \subset \mathcal{X} \to \mathcal{X}^*$$

We know that

$$D(H_U) = \{\psi \in D(H^*) \,|\, i(\mathbb{I}+U)\boldsymbol{\gamma}\psi = (\mathbb{I}-U)\boldsymbol{\mu}\psi\}$$

By projecting on $\mathcal{X}$ and $\mathcal{X}^\perp$ the equation $i(\mathbb{I}+U)\boldsymbol{\gamma}\psi = (\mathbb{I}-U)\boldsymbol{\mu}\psi$, one gets

$$D(H_U) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in \mathcal{X},\, i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

Since $(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} = \Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}$, for all $\psi \in D(H^*)$, we have that

$$D(H_U) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in \mathcal{X},\, i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}.$$

Again by Lemma 14, one has that

$$D(H_U) = \left\{\psi \in D(H^*) \,|\, \boldsymbol{\gamma}\psi \in D(\Lambda L),\, i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}$$

and thus

$$D(H_U) = D(H_{(\mathcal{X},L)}).$$ □

5.8 The Cayley transform: supplemental results

Let us recall some basic facts about the Cayley transform of self-adjoint operators. For further details see [Rud91].

Definition 8. Let $A : D(A) \subset \mathscr{H} \to \mathscr{H}$ be a self-adjoint operator. We define the *Cayley transform* of A, denoted by $\mathscr{C}(A)$, as follows

$$\mathscr{C}(A) = (A - i\mathbb{I})(A + i\mathbb{I})^{-1},$$

where $\mathbb{I}$ is the identity operator on $\mathscr{H}$.
Conversely, let $U \in \mathrm{U}(\mathscr{H})$ and assume that 1 is not an eigenvalue of U. We define the *inverse Cayley transform* of U, denoted by $\mathscr{C}^{-1}(U)$, as follows

$$\mathscr{C}^{-1}(U) = i(\mathbb{I}+U)(\mathbb{I}-U)^{-1}.$$

Proposition 13 ([Rud91])**.** *Let $A : D(A) \subset \mathscr{H} \to \mathscr{H}$ be a self-adjoint operator. Then*

1. $\mathscr{C}(A) \in \mathrm{U}(\mathscr{H})$;
2. $\mathbb{I} - \mathscr{C}(A)$ *is injective;*
3. $\mathrm{Ran}(\mathbb{I} - \mathscr{C}(A)) = D(A)$;
4. *For all $\phi \in D(A)$,*

$$A\phi = i(\mathbb{I} + \mathscr{C}(A))(\mathbb{I} - \mathscr{C}(A))^{-1}\phi = \mathscr{C}^{-1}(\mathscr{C}(A))\phi.$$

5. *Moreover if $U \in \mathrm{U}(\mathscr{H})$ such that 1 is not an eigenvalue of U then*

$$\mathscr{C}^{-1}(U) : \mathrm{Ran}(\mathbb{I} - U) \to \mathscr{H}$$

is a self-adjoint operator and $\mathscr{C}(\mathscr{C}^{-1}(U)) = U$.

Lemma 14. *Let $A : D(A) \subset \mathscr{H} \to \mathscr{H}$ be a self-adjoint operator and*

$$\mathcal{G}(A) = \{(u, Au) \in \mathscr{H} \times \mathscr{H} \,|\, u \in D(A)\}$$

be its graph. Let

$$\Theta(A) = \{(\phi, \psi) \in \mathscr{H} \times \mathscr{H} \,|\, i(\mathbb{I} + \mathscr{C}(A))\,\phi = (\mathbb{I} - \mathscr{C}(A))\,\psi\}.$$

Then $\mathcal{G}(A) = \Theta(A)$.

Proof. Notice first that the inclusion $\mathcal{G}(A) \subset \Theta(A)$ follows immediately from property 4 of Proposition 13. We need to show that $\Theta(A) \subset \mathcal{G}(A)$.
Fix $(\phi, \psi) \in \mathscr{H} \times \mathscr{H}$ such that

$$i(\mathbb{I} + \mathscr{C}(A))\,\phi = (\mathbb{I} - \mathscr{C}(A))\,\psi. \tag{5.16}$$

Observe that

$$\mathbb{I} - \mathscr{C}(A) = 2i(A + i\mathbb{I})^{-1} \quad \text{and} \quad \mathbb{I} + \mathscr{C}(A) = 2A(A + i\mathbb{I})^{-1}.$$

Plugging these expressions in equation (5.16) we obtain:

$$A\,(A + i\,\mathbb{I})^{-1}\phi = (A + i\,\mathbb{I})^{-1}\psi.$$

The right hand side belongs to $D(A)$, thus also the left hand side belongs to $D(A)$. Then we can multiply both sides by $A + i\,\mathbb{I}$, obtaining

$$\psi = (A + i\,\mathbb{I})\,A\,(A + i\,\mathbb{I})^{-1}\phi.$$

Since $(A + i\,\mathbb{I})^{-1}\phi \in D(A)$ and $A\,(A + i\,\mathbb{I})^{-1}\phi \in D(A)$, it follows that $(A + i\,\mathbb{I})^{-1}\phi \in D(A^2)$. The operators $(A + i\,\mathbb{I})$ and A commute on $D(A^2)$ and we get that

$$\psi = A\phi,$$

and thus $(\phi, \psi) \in \mathcal{G}(A)$. □

Conclusions

In this dissertation we have tried to motivate the importance of quantum boundary conditions as an effective tool for describing quantum bounded systems.

In Chapter 1 we gave an overview on the range of physical phenomena where quantum boundary conditions have proved their essential usefulness. We reviewed the Casimir effect, and discussed how the force between the plates could be attractive, repulsive or even zero according to the boundary conditions chosen. We analyzed the quantum Hall effect, where the resulting edge current can be explained in terms of chiral boundary conditions.

Interesting perspectives in quantum gravity were exposed making use of models of topology change, which may occur when energies at the Planck scale are involved. Modifications of the space time texture were implemented in terms of boundary conditions change at the level of Hilbert spaces.

In addition to that, we also analyzed the Aharonov-Bohm effect and compared the resulting cross sections in light of different boundary conditions imposed on the solenoid.

We understood how boundary conditions play a principal role in the study of precise physical situations, since they represent our link between the actual system and the mathematical model. In fact, we were able to give a physical interpretation of boundary conditions based on scattering by plane waves, and understood their different physical interpretations.

In the whole thesis we lingered over the case of a free nonrelativistic quantum particle inside a cavity and analyzed different emerging physical situations.

In Chapter 2 we proved the existence of a geometric phase for a quantum particle in a box with moving walls with the prescription of suitable boundary

conditions. First of all we needed to specify the domain of definition of the Hamiltonian. Since the walls were not fixed, the problem consisted of a family of Hamiltonians defined over changing domains. This is already a complicated problem that needs to be well posed. Moreover we needed to choose a particular family of self-adjoint extensions.

After having studied its spectral decomposition we computed the one-form connection associated to our problem and its circulation on a certain closed path in the parameter space. A technical problem shown up: the coefficients of the one-form needed to be handled with care, since divergent contributions arose from the boundary and a prescription on how to *renormalize* the result was indeed necessary.

In correspondence of different values of the parameter labelling the boundary conditions, we were able to associate spectral decompositions of different kind. In the previous discussion a non degenerate spectrum was assumed, so that an Abelian phase was found. On the other hand there were some cases where the spectrum could be degenerate and we considered the Wilczek-Zee phase, which is a natural non-abelian generalization of the Berry phase.

All the considerations were made for a one-dimensional system. An interesting perspective would be to exploit further degrees of freedom, which naturally emerge when considering regions in higher dimensional spaces. Moreover, the particle considered was spinless. Interestingly, one could check what happens when a spin is introduced because interactions between the spin degrees of freedom and the boundary may reveal some new results.

In the next chapter, we left the adiabatic evolution and moved on to a different dynamical situation. We considered the case of rapidly alternating boundary conditions for our particle in a cavity. This evolution à la Trotter involved two different boundary conditions rapidly interchanging. We proved that the limiting dynamics could be obtained from the boundary conditions we started with and we determined the corresponding composition law.

We started with the one-dimensional case, introducing an alternative parametrization of the self-adjoint realizations in terms of spectral projections. Afterwards we moved on to higher dimensions were further difficulties were unavoidably encountered. The problem was solved and examples were pro-

vided.

Up to now it is not known how to consider general dynamical evolutions in the space of boundary conditions. It is only known how to treat special kinds of dynamics. Interestingly enough, it would be challenging to adventure on more general evolutions, trying to highlight, at least, and circumscribe the obstructions.

In Chapter 5 we understood how to generate boundary conditions starting from a quantum system on a manifold without boundaries. We focused on two different approaches. Indeed, we first considered the process of generating boundaries from a manifold without boundary by means of a group action. In particular, we considered the case of a circle, which was transformed into a segment, where Dirichlet and Neumann boundary conditions were implemented. Moreover, we investigated another way of generating more general boundary conditions, e.g. Robin boundary conditions, by changing the metric near the boundaries.

Eventually, we explored this problem in another direction. Indeed, instead of quotienting the base manifold, we folded it in two distinct copies of a manifold with boundary. We considered the case of a free quantum particle on a line, which was folded into two copies of the half-line. In this manner we were able to unitarily map the problem into a larger space, involving an auxiliary space. Boundary conditions emerged on the half-line at the cost of introducing the spin for our particle. Similarly we studied the case of a particle on the unit circle, which can be folded into two copies of a segment, with the consequent spin degrees of freedom. Eventually we discussed the link between self-adjointness and entanglement generation, and tried to give a perspective for further generalizations of the problem.

In the end, in the last chapter, we based on solid mathematical grounds the results obtained in the previous sections. In particular, we stressed the one-to-one correspondence between the set of self-adjoint extensions for the Hamiltonian describing the free quantum particle in the cavity and the set of unitary operators acting on the border.

We compared this result with other parametrisations well known in literature and tried to compare the pros and cons deriving from the different

parametrizations. All the results discussed were accompanied by the respective proofs.
In this case it would be interesting to extend the aforementioned parametrization to general elliptic operators and Dirac operators, for further applications to other physical situations.

Bibliography

[AA87] Y. Aharonov and J. Anandan, "Phase Change during a Cyclic Quantum Evolution", *Phys. Rev. Lett.* 58 (1987), pp. 1593–1596.

[AB59] Y. Aharonov and D. Bohm, "Significance of electromagnetic potentials in quantum theory", *Phys. Rev.* 115 (1959), pp. 485–491.

[AE99] J. E. Avron and A. Elgart, "Adiabatic theorem without a gap condition", *Commun. Math, Phys.* 203 (1999).

[AF02] R.A. Adams and J.J. Fournier, *Sobolev Spaces.Second Edition*, Academic Press, New York, 2002.

[AFM03] D.T. Alves, C. Farina, and P. A. Maia Neto, "Dynamical Casimir effect with Dirichlet and Neumann boundary conditions", *J. Phys. A: Math. Gen.* 36 (2003).

[AG93] N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space*, ed. by New York Dover Publications, 1993.

[AGM06] M. Asorey, D. García-Alvarez, and J.M. Muñoz-Castañeda, "Casimir effect and global theory of boundary conditions", *J. Phys. A: Math. Gen.* 39 (2006).

[AGM15] M. Asorey, D. García-Alvarez, and J.M. Muñoz-Castañeda, "Boundary Effects in Bosonic and Fermionic Field Theories", *Int. J. Geom. Methods Mod. Phys.* 12 (2015).

[AIM05] M. Asorey, A. Ibort, and G. Marmo, "Global Theory of Quantum Boundary Conditions and Topology Change", *Int. J. Mod. Phys. A* 20 (2005), p. 1001.

[AIM15] M. Asorey, A. Ibort, and G. Marmo, "The topology and geometry of self-adjoint and elliptic boundary conditions for Dirac and Laplace operators", *Int. J. Geom. Methods Mod. Phys.* 12 (2015).

[Akk+98] E. Akkermans, J. E. Avron, R. Narevich, and R. Seiler, "Boundary conditions for bulk and edge states in quantum Hall systems", *Eur. Phys. J. B* 1 (1998), p. 117.

[AM07] W. Arendt and R. Mazzeo, "Spectral properties of the Dirichlet-to-Neumann operator on Lipschitz domains", *Ulmer Seminare* 12 (2007).

[AM11] M. Asorey and J.M. Muñoz-Castañeda, "Vacuum Boundary Effects", *Int. J. Theor. Phys.* 50 (2011), pp. 2211–2221.

[AM13] M. Asorey and J.M. Muñoz-Castañeda, "Attractive and repulsive Casimir vacuum energy with general boundary conditions", *Nuclear Phys. B* 874 (2013).

[APS75] M. F. Atiyah, V. K. Patodi, and I. M. Singer, "Spectral asymmetry and Riemannian geometry I", *Math. Proc. Camb. Phil. Soc.* 77 (1975).

[Arn97] V.I. Arnol'd, *Mathematical Methods of Classical Mechanics.Second Edition*, ed. by Springer, vol. 60, Graduate Text in Mathematics, 1997.

[Aso+12] M. Asorey, A.P. Balachandran, I.P. Marmo G. Costa e Silva, A.R. de Queiroz, P. Teotonio-Sobrinho, and S. Vaidya, *Quantum Physics and Fluctuating Topologies: Survey.* 2012, arXiv: `1211.6882 [hep-th]`.

[Aso+13] M. Asorey, P. Facchi, G. Marmo, and S. Pascazio, "A Composition law for boundary conditions", *J. Phys. A: Math. Theor.* 46 (2013), p. 102001.

[AT98] R. Adami and A. Teta, "On the Aharonov-Bohm Hamiltonian", *Lett. Math. Phys.* 43 (1998), p. 43.

[Bal+83] A.P. Balachandran, G. Marmo, B. Skagerstan, and A. Stern, *Gauge theories and fiber bundles: Applications to particle dynamics*, vol. 188, Springer Lecture Notes in Physics, 1983.

[Bal+91] A.P. Balachandran, G. Marmo, B. Skagerstan, and A. Stern, *Classical topology and quantum states*, World Scientific, 1991.

[Bal+95] A.P. Balachandran, G. Bimonte, G. Marmo, and A. Simoni, "Topology change and quantum physics", *Nucl.Phys.* 446 (1995), p. 299.

[Bar93] G. Barton, *New aspects of the Casimir effect: fluctuations and radiative reaction.Cavity Quantum Electrodynamics (Supplement: Advances in Atomic, Molecular and Optical Physics)*, Academic Press, 1993.

[BD87] T. Bitter and D. Dubbers, "Manifestation of Berry's Topological Phase in Neutron Spin Rotation", *Phys. Rev. Lett.* 3 (1987).

[Ber+79] M. V. Berry, N. L. Balazs, M. Tabor, and A. Voros, "Quantum maps," *Ann. Phys.* 122 (1979), p. 26.

[Ber84] M.V. Berry, "Quantal phase factors accompanying adiabatic changes", *Proc. R. Soc. Lond. A* 292 (1984), pp. 45–47.

[BF28] M. Born and V. Fock, "Beweis des Adiabatensatzes", *Zeitschrift für Physik* 51.3-4 (1928), pp. 165–180.

[BGM71] M. Berger, P. Gauduchon, and E. Mazet, *Le Spectre d'une Variete Riemannienne*, Springer-Verlag, Berlin, 1971.

[BGP08] J. Brüning, V. Geyler, and K. Pankrashkin, "Spectra of self-adjoint extensions and applications to solvable Schrödinger operators", *Rev. Math. Phys.* 20 (2008).

[Bir56] M.S. Birman, "On the theory of self-adjoint extensions of positive definite operators", *Mat. Sbornik* 38 (1956).

[Bla+60] W. Black, J. G. V. De Jongh, J.Th.G. Overbeek, and M. J. Sparnaay, "Measuraments of retarded van Der Waals' forces", *Trans. Faraday Soc.* 56 (1960).

[Boh+03] A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, and J. Zwanziger, *The Geometric Phase in Quantum Systems*, ed. by Berlin Springer, 2003.

[BR03] O. Bratteli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics*, vol. 1, Springer Verlag, 2003.

[Bre10] H. Brezis, *Functional Analysis, Sobolev Spaces and Partial Differential Equations*, Springer, Berlin, 2010.

[BW84] M.V. Berry and M. Wilkinson, "Diabolical points in the spectra of triangles", *Proc. R. Soc. Lond. A* 392 (1984), pp. 15–43.

[Cal39] J.W. Calkin, "Abstract symmetric boundary conditions", *Trans. of the Amer. Math. Soc.* 45.3 (1939), pp. 369–442.

[Cas+79] G. Casati, B. V. Chirikov, J. Ford, and F. M. Izrailev, *Stochastic Behaviour in Classical and Quantum Hamiltonian Systems*, edited by G. Casati and J. Ford, Lecture Notes in Physics Vol. 93, Springer-Verlag, 1979.

[Cas48] H. B. G. Casimir, "On the attraction between two perfectly conducting plates", *Proc. K. Ned. Akad. Wet.* 51 (1948).

[Cat+01] F.S. Cataliotti, S. Burger, C. Fort, P. Maddaloni, F. Minardi, A. Trombettoni, A. Smerzi, and M. Inguscio, "Josephson junction arrays with Bose-Einstein condensates", *Science* 293 (2001).

[CFT01] T. Cheon, T. Fülop, and I. Tsutsui, "Symmetry, Duality, and Anholonomy of Point Interactions in One Dimension", *Ann. Phys.* 294 (2001), p. 25.

[Cha31] R.G. Chambers, "Shift of an Electron Interference Pattern by Enclosed Magnetic Flux", *Phys. Rev. Lett.* 5 (1931), pp. 3–5.

[CJ04] D. Chruściński and A. Jamiołkowski, *Geometric Phases in Classical and Quantum Mechanics*, ed. by Boston Birkäuser, 2004.

[Del15] G. Dell'Antonio, *Lectures on the Mathematics of Quantum Mechanics I*, ed. by Amsterdam Atlantis Press, 2015.

[DF15] S. Di Martino and P. Facchi, "Quantum systems with time-dependent boundaries", *Int. J. Geom. Methods Mod. Phys.* 12 (2015).

[Di +16] S. Di Martino, F. Anzà, P. Facchi, A. Kossakowski, G. Marmo, A. Messina, B. Militello, and S. Pascazio, "A quantum particle in a box with moving walls", *J. Phys. A: Math. Theor.* 46 (2016), p. 365301.

[Dir31a] P.A.M. Dirac, "Quantised Singularities in the Electromagnetic Field", *Proc. Roy. Soc. A* 133 (1931).

[Dir31b] P.A.M. Dirac, "Quantised Singularities in the Electromagnetic Field", *Proceedings of the Royal Society A* 133.60 (1931).

[DJC14] S. Deffner, C. Jarzynski, and A. del Campo, "Classical and Quantum Shortcuts to Adiabaticity for Scale-Invariant Driving", *Phys. Rev. X* 4 (2014).

[DS98] L. Dabrowski and P. Stovicek, "Aharonov-Bohm effect with δ-type interaction", *J. Math. Phys.* 39 (1998), p. 47.

[ENZ11] P. Exner, H. Neidhardt, and V. A. Zagrebnov, "Remarks on the Trotter-Kato product formula for unitary groups", *Integr. Equ. Oper. Theory* 69 (2011), p. 451.

[ESV02] P. Exner, P. St'ovicek, and P. Vytras, "Generalized boundary conditions for the Aharonov-Bohm effect combined with a homogeneous magnetic field", *J. Math. Phys.* 43 (2002), p. 2151.

[Eva10] L.C. Evans, *Partial Differential Equations*, Amer. Mathematical Society, 2010.

[Eze08] Z. F. Ezewa, "Quantum Hall Effects (Second Edition)" (2008).

[Fab02] M. Fabinger, "Higher-dimensional quantum Hall effect in string theory", *J. High Energy Phys.* 5 (2002), p. 37.

[Fac+16] P. Facchi, G. Garnero, G. Marmo, and J. Samuel, "Moving Walls and geometric phases", *Ann. Phys.* 372 (2016).

[Fac+17] P. Facchi, G. Garnero, G. Marmo, J. Samuel, and S. Sinha, "Boundaries without boundaries" (2017), arXiv: 1710.10901.

[FGL17a] P. Facchi, G. Garnero, and M. Ligabò, "Quantum Cavities with alternating boundary conditions" (2017), arXiv: 1710.10893.

[FGL17b] P. Facchi, G. Garnero, and M. and Ligabò, "Self-adjoint extensions and unitary operators on the boundary", *Lett. Math. Phys.* (2017), DOI: 10.1007/s11005-017-1001-8.

[FL10] P. Facchi and M. Ligabò, "Quantum Zeno effect and dynamics", *J. Math. Phys.* 51 (2010), p. 022103.

[FLS70] R.P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics*, Addison Wesley Longman, 1970.

[Fol09] G. B. Folland, *Fourier Analysis and its Applications*, Amer. Mathematical Society, 2009.

[Fol99] G. B. Folland, *Real Analysis: Modern Techniques and Their Applications*, Wiley, New York, 1999.

[Fow+66] A.B. Fowler, F.F. Fang, W.E. Howard, and P.J. Stiles, "Magneto-Oscillatory Conductance in Silicon Surfaces", *Phys. Rev. Lett.* 16 (1966), p. 901.

[FP08] P. Facchi and S. Pascazio, "Quantum Zeno dynamics: mathematical and physical aspects", *J. Phys. A: Math. Theor.* 41 (2008), p. 493001.

[FT01] T. Fülop and I. Tsutsui, "Möbius structure of the spectral space of Schrödinger operators with point interaction", *J. Math. Phys.* 42 (2001), p. 56.

[GER09] G. Granger, J. P. Eisenstein, and J. L. Reno, "Observation of chiral heat transport in the quantum Hall regime", *Phys. Rev. Lett.* 102 (2009), p. 086803.

[GFL10] S. Graffi, P. Facchi, and M. Ligabò, "The classical limit of the quantum Zeno effect", *J. Phys. A: Math. Theor.* 43 (2010), p. 032001.

[GM11] F. Gesztesy and M. Mitrea, "A description of all self-adjoint extensions of the Laplacian and Kreĭn-type resolvent formulas on non-smooth domains", *J. Anal. Math.* 113 (2011).

[Gre98] M. Greiter, "Quantum Hall quarks or short distance physics of quantized Hall fluids", *Int. J. Mod. Phys. A* 13 (1998), p. 1293.

[Gru09] G. Grubb, *Distributions and Operators*, Springer-Verlag, Berlin, 2009.

[Gru68] G. Grubb, "A characterization of the non-local boundary value problems associated with an elliptic operator", *Ann. Scuola Norm. Sup. Pisa* 22 (1968).

[Gru74] G. Grubb, "Properties of normal boundary value problems for elliptic even-order systems", *Ann. Scuola Norm. Sup. Pisa Ser. IV* 1 (1974), pp. 1–61.

[Hag90] C. R. Hagen, "Aharonov- Bohm scattering amplitude", *Phys. Rev. D* 41 (1990), p. 2015.

[Hal82] B.I. Halperin, "Quantized Hall conductance, current-carrying edge states and the existence of extended states in a two-dimensional disordered potential", *Phys.Rev. B* 25 (1982), p. 2185.

[HL63] G. Herzberg and H.C. Longuet-Higgins, "Intersection of potential energy-surfaces in polyatomic molecules", *Disc. Farad. Soc.* 35 (1963).

[HOR04] F. W. Hehl, Y. N. Obukhov, and B. Rosenow, "Is the quantum Hall effect influenced by the gravitational field?", *Phys. Rev. Lett.* 93 (2004), p. 096804.

[Hor63] L. Hörmander, *Linear Partial Differential Operators*, Springer-Verlag, Berlin, 1963.

[ILP15a] A. Ibort, F. Lledo, and J.M. Perez-Pardo, "On self-adjoint extensions and symmetries in Quantum Mechanics", *Ann. H. Poinc.* 16 (2015).

[ILP15b] A. Ibort, F. LLedó, and J.M. Pérez-Pardo, "Self-adjoint extensions of the Laplace-Beltrami operator and unitaries at the boundary", *J. Funct. Anal.* 268 (2015), pp. 634–670.

[ILP15c] A. Ibort, F. Lledó., and J.M. Pérez-Pardo, "Self-adjoint extensions of the Laplace-Beltrami operator and unitaries at the boundary", *J. Funct. Anal.* 268 (2015).

[IMP14] A. Ibort, G. Marmo, and J.M. Perez-Pardo, "Boundary dynamics driven entaglement", *J. Phys. A: Math. Theor.* 47 (2014).

[IMT96] K. Ishikawa, N. Maeda, and K. Tadaki, "Integer quantum Hall effect with realistic boundary conditionn: exact quantization and breakdown", *Phys. Rev. B* 54 (1996), p. 17819.

[Jac98] J.D. Jackson, *Classical Electrodynamics*, Wiley, 1998.

[JL00] G. W. Johnson and M. L. Lapidus, *The Feynman integral and Feynman's operational calculus*, Oxford University Press, New York, 2000.

[Jos11] J. Jost, *Riemannian Geometry and Geometric Analysis*, ed. by Springer, 2011.

[Jos62] B.D. Josephson, "Possible new effects in superconductive tunneling", *Phys. Lett.* 1 (1962), p. 251.

[Kac66] M. Kac, "Can one hear the shape of a drum?", *American Mathematical Monthly* 73 (1966), pp. 1–21.

[Kat50] T. Kato, "On the Adiabatic Theoreom of Quantum Mechanics", *J. Phys. Soc. of Jpn.* 5.6 (1950), pp. 435–439.

[Kat66] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin, 1966.

[KDP80] K. von Klitzing, G. Dorda, and M. Pepper, "New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistence", *Phys. Rev. Lett.* 45 (1980), p. 494.

[KE85] K. von Klitzing and G. Ebert, "Application of the Quantum Hall Effect in Metrology", *Metrologia* 21 (1985), p. 11.

[Kim10] J. E. Kim, "A review on axions and the strong CP problem", *AIP Conf.Proc.* 1200 (2010), pp. 83–92.

[Kli05] K. von Klitzing, "25 Years of Quantum Hall Effect (QHE) A Personal View on the Discovery, Physics and Applications of this Quantum Effect", *The Quantum Hall Effect, Poincaré Seminar 2004* (2005), pp. 1–21.

[Kre47] M. Kreĭn, "The theory of self-adjoint extensions of semi-bounded Hermitian transformations and its applications.", *I. Rec. Math. [Mat. Sbornik] N.S.* 20 (1947).

[Lam97] S. K. Lamoreaux, "Demonstration of the Casimir Force in the 0.6 to 6μm range", *Phys. Rev. Lett.* 78.5 (1997).

[Lap82] M. L. Lapidus, "The problem of the Trotter-Lie formula for unitary groups of operators. Séminaire Choquet: Initiation à l'Analyse.", *Publ. Math. Univ. Pierre et Marie Curie (Paris IV)* 46 (1982), p. 1701.

[Lau81] R.B. Laughlin, "Quantized Hall conductivity in two dimensions", *Phys. Rev. B* 23 (1981), p. 5632.

[Lau83] R.B. Laughlin, "Anomalous Quantum Hall Effect: An Incompressible Quantum Fluid with Fractionally Charged Excitations", *Phys. Rev. Lett.* 50 (1983), p. 1395.

[Lee02] J. M. Lee, *Introduction to Smooth Manifolds*, ed. by Springer, 2002.

[LL77] L. D. Landau and E. M. Lifschitz, *Quantum Mechanics: Non-relativistic Theory. Course of Theoretical Physics.* Pergamon Press, 1977.

[LM72] J. L. Lions and E. Magenes, *Non-Homogeneous Boundary Value Problems and Applications I*, Springer-Verlag, Berlin, 1972.

[Mac90] A. H. MacDonald, "Edge states in the fractional quantum Hall effect regime", *Phys. Rev. Lett.* 64 (1990), p. 220.

[MB62] G. Mollenstedt and W. Bayh, "Kontinuierliche Phasenverschiebung von Elektronenwellen im kraftfeldfreien Raum durch das Vektorpotential eines Solenoids", *Physikalische Blatter* 18 (1962).

[MCP09] J. N. Munday, F. Capasso, and V.A. Parsegian, "Measured long-range repulsive Casimir-Lifshitz forces", *Nature* 457.170 (2009).

[Mes61] A Messiah, *Quantum Mechanics*, ed. by Amsterdam North-Holland, 1961.

[MF94] Stone M. and M. P. A. Fisher, "Laughlin states at the edge", *Int. J. Mod. Phys.* B8 (1994), p. 2539.

[Min+06a] B. Mintz, C. Farina, P. A. Maia Neto, and R. B. Rodrigues, "Casimir forces for moving boundaries with Robin conditions", *J. Phys. A: Math. Gen.* 39 (2006), p. 6559.

[Min+06b] B. Mintz, C. Farina, P. A. Maia Neto, and R. B. Rodrigues, "Particle creation by a moving boundary with a Robin boundary condition", *J. Phys. A: Math. Gen.* 39 (2006), p. 11325.

[MR98] U. Mohideen and A. Roy, "Precision Measurement of the Casimir Force from 0.1 to 0.9μm", *Phys. Rev. Lett.* 81 (1998).

[Myu99] Y. S. Myung, "BTZ black hole and quantum Hall effect in the bulk-boundary dynamics", *Phys. Rev. D* 59 (1999), p. 044028.

[NB09] Y.V. Nazarov and Y.M. Blanter, *Quantum Transport: Introduction to Nanoscience*, Cambridge University Press, 2009.

[Neu55] J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, 1955.

[NK98] Q. Niu and L. Kleinman, "Spin-wave Dynamics in Real Crystals", *Phys. Rev. Lett.* 80.(2205) (1998).

[Oli08] C.R. de Oliveira, *Intermediate Spectral Theory and Quantum Dynamics*, ed. by Boston Birkäuser, Progress in Mathematical Physics, 2008.

[OP08] C. R. de Oliveira and M. Pereira, "Mathematical justification of the Aharonov-Bohm Hamiltonian", *J. Stat. Phys.* 133 (2008), p. 1175.

[OP10] C. R. de Oliveira and M. Pereira, "Scattering and self-adjoint extensions of the Aharonov-Bohm Hamiltonian", *J.Phys. A: Math. Theor.* 43 (2010), p. 354011.

[Paa+09] F. G. Paauw, A. Fedorov, C. J. P. M. Harmans, and J. E. Mooij, "Tuning the Gap of a Superconducting Flux Qubit", *Phys. Rev. Lett.* 102 (2009), p. 090501.

[Pan56] S. Pancharatnam, "Generalized Theory of Interference and its Applications", *Proc. Indian Acad. Sci.* 5 (1956).

[Pec08] R. D. Peccei, *The Strong CP Problem and Axions*, vol. 741, Lect. Notes Phys. Springer-Verlag, 2008.

[Pei79] R. Peierls, *Surprises in Theoretical Physics*, Princeton University Press, 1979.

[PMG86] G. Plunien, B. Müller, and W. Greiner, "The Casimir Effect", *Phys. Rep.* 134 (1986), pp. 87–193.

[Poi+11] W. Poirier, F. Schopfer, J. Guignard, O. Thévenot, and P. Gournay, "Application of the quantum Hall effect to resistance metrology", *C. R. Physique* 12 (2011), p. 347.

[Pol+09] S. Poletto, F. Chiarello, M. G. Castellano, J. Lisenfeld, A. Lukashenko, C. Cosmelli, G. Torrioli, P. Carelli, and A. V. Ustinov, "Coherent oscillations in a superconducting tunable flux qubit manipulated without microwaves", *New Journal of Physics* 11 (2009), p. 013009.

[Pos03] A. Posilicano, "Self-Adjoint Extensions by Additive Perturbations", *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* 2 (2003).

[Pos08] A. Posilicano, "Operators and Matrices", *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* 2 (2008).

[PR11] K. Pankrashkin and S. Richard, "Spectral and scattering theory for the Aharonov-Bohm operators", *Rev. Math. Phys.* 23 (2011), p. 53.

[PVK98] V. Privman, I. D. Vagner, and G. Kventsel, "Quantum computation in quantum Hall systems", *Phys. Lett. A* 239 (1998), p. 141.

[QT87] Niu Q. and D.J. Thouless, "Quantum Hall effect with realistic boundary conditions", *Phys. Rev. B* 35 (1987), p. 2188.

[RB85] M. Robnik and M.V. Berry, "Classical billiards in magnetic fields", *J. Phys. A* 18 (1985), p. 1361.

[RS75] M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Academic Press, 1975.

[Rud91] W. Rudin, *Functional Analysis. Second Edition*, ed. by New York McGraw-Hill Publ.Comp, 1991.

[Rui83] S. N. M. Ruijsenaars, "The Aharonov-Bohm effect and scattering theory", *Ann. Phys.* 146 (1983), p. 1.

[SA73] E.S. Sabisky and C.H. Anderson, "Verification of the Lifshitz Theory of the van der Waals Potential Using Liquid-Helium Films", *Phys. Rev. A* 7.790 (1973).

[Sa86] J. Schelter and al., "The Aharonov-Bohm effect in graphene rings", *Solid State Comm.* 152 (1986).

[Sak93] J.J. Sakurai, *Modern Quantum Mechanics*, ed. by Addison Wesley, 1993.

[SB88] J. Samuel and R. Bhandari, "General Setting for Berry's Phase", *Phys. Rev. Lett.* 60.23 (1988), pp. 2339–2342.

[Sci] Royal Swedish Academy of Science, URL: `https://www.nobelprize.org/nobel_prizes/physics/laureates/1998/press.html`.

[SE06] A. Saharian and G. Esposito, "Casimir effect with non-local boundary conditions", *J.Phys. A: Math. Gen.* 39 (2006), p. 5233.

[Sil66] A. van Silfhout, *Proc. Kon. Ned. Akad. Wet.* B 69.501 (1966).

[Sim83] B. Simon, "Holonomy, the Quantum Adiabatic Theorem, and Berry's Phase", *Phys. Rev. Lett.* 51.24 (1983), pp. 137–140.

[Spa57] M. J. Sparnaay, "Attractive forces between flat plates", *Nature* 180 (1957).

[SS10] A. Saharian and M. R. Setare, "Casimir effect for curved boundaries in Robertson-Walker spacetime", *Class. Quant. Grav.* 27 (2010), p. 225009.

[SW03] A. Shapere and F. Wilczek, *Geometric Phases in Physics*, ed. by World Scientific, Advanced Series in Mathematical Physics, 2003.

[SWX12] A.D. Shapere, F. Wilczek, and Z. Xiong, *Models of Topology Change*, 2012, arXiv: `1210.3545`.

[Ta82] A. Tonomura and al., "Observation of Aharonov-Bohm effect by electron holography", *Phys. Rev. Lett.* 48 (1982).

[Ta86] A. Tonomura and al., "Evidence for Aharonov-Bohm effect with magnetic field completely shielded from electron wave", *Phys. Rev. Lett.* 56 (1986).

[TFC00] I. Tsutsui, T. Fülop, and T. Cheon, "A free particle on a circle with point interaction", *Phys. Lett. A* 264 (2000), p. 366.

[Tho93] D.J. Thouless, "Edge voltages and distributed currents in the quantum Hall effect", *Phys. Rev. Lett.* 71 (1993), p. 1873.

[Tre06] F. Treves, *Basic Linear Partial Differential Equations*, ed. by New York Dover, 2006.

[Tro59] H. F. Trotter, "On the product of semi-groups of operators", *Proc. Amer. Math. Soc.* 10 (1959), p. 545.

[Tro78] H. F. Trotter, "Trotter's product formula for an arbitrary pair of self-adjoint contraction semigroup", *Topics in functional analysis, Adv. in Math. Suppl. Stud.* 3 (1978), p. 185.

[TW68] D. Tabor and R.H.S. Winterton, "Surface Forces: Direct Measurement of Normal and Retarded van der Waals Forces", *Nature* 219 (1968).

[Vis63] M.I. Vishik, "On general boundary problems for elliptic differential equations", *Amer. Math. Soc. Transl.: II* 24 (1963), pp. 107–172.

[Wei05] S. Weinberg, *The Quantum theory of Fields*, Cambridge University Press, 2005.

[Wen90] X. G. Wen, "Electrodynamical properties of gapless edge excitations in the fractional quantum Hall states", *Phys. Rev. Lett.* 64 (1990), p. 2206.

[Wen91] X. G. Wen, "Edge excitations in the fractional quantum Hall states at general filling fractions", *Mod. Phys. Lett. B* 5 (1991), p. 39.

[Wen92] X. G. Wen, "Theory of the edge states in fractional quantum Hall effects", *Int. J. Mod. Phys.* B6 (1992), p. 1711.

[Wik] Wikipedia, URL: `https://it.wikipedia.org/wiki/Effetto_Hall`.

[Wil+10] C.M. Wilson, T. Duty, M. Sandberg, F. Persson, V. Shumeiko, and P. Delsing, "Photon Generation in an Electromagnetic Cavity with a Time-Dependent Boundary", *Phys. Rev. Lett.* 105 (2010), p. 233907.

[WZ83] F. Wilczek and A. Zee, "Appearance of gauge structure in simple dynamical systems", *Phys. Rev. Lett.* 52 (1983), pp. 2111–2114.

[ZH01] S.C. Zhang and J. Hu, "A four dimensional generalization of the quantum Hall effect", *Science* 294 (2001), p. 823.

Acknowledgements

I would like to express my sincere and profound gratitude to my supervisor, prof. Paolo Facchi for his expert guidance and constant encouragement. Without his patience and passion, this work would have not seen the light.
Let me thank prof. Giuseppe Marmo and prof. Saverio Pascazio for the interesting and stimulating discussions, they let me take part to during these three years.
I would like also to thank prof. Hiromichi Nakazato and prof. Kazuya Yuasa for their kind hospitality at Waseda University, Tokyo and for showing me their way of doing scientific research.
I would like to extend my thanks to prof. Alberto Ibort and prof. Manuel Asorey for their kind hospitality at ICMAT, Madrid and the University of Zaragoza. The spanish stay has been fundamental both from a scientific and a personal point of view.
Let me thank Giuseppe Florio and Marilena Ligabò for their priceless suggestions and advice. It has been a pleasure both discussing ideas with them and enjoying scientific conferences.
Let me also add my gratitude to Sara Di Martino e Fabio Deelan Cunden, for introducing to the PhD world from the PhD students' perspective.
Last but not the least, I would like to thank my family and my friends for supporting me and overwhelming me with their love during my ups and downs, through my good and bad days.